NORTH-HOLLAND

Largest j-Simplices in d-Cubes: Some Relatives of the Hadamard Maximum Determinant Problem

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ABSTRACT

This paper studies the computationally difficult problem of finding a largest j-dimensional simplex in a given d-dimensional cube. The case in which $j = d$ is of special interest, for it is equivalent to the Hadamard maximum determinant problem; it has been solved for infinitely many values of d but not for $d = 14$. (The subcase in which $j = d \equiv 3 \pmod 4$ subsumes the famous problem on the existence of Hadamard matrices.) The known results for the case $j = d$ are here summarized and used, but the main focus is on fixed small values of j. When $j = 1$, the problem is trivial, and when $j = 2$ or $j = 3$ it is here solved completely (i.e., for all d). Beyond that, the

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LINEAR ALGEBRA AND ITS APPLICATIONS 241–243:519–598 (1996)

0024-3795/96/$15.00
SSDI 0024-3795(95)00541-X

results are fragmentary but numerous, and they lead to several attractive conjectures. Some other problems involving simplices in cubes are mentioned, and the relationship of largest simplices to D-optimal weighing designs is discussed.

INTRODUCTION

The setting for everything in this paper is a finite-dimensional Euclidean space $\mathbb{R}^d$ whose origin is denoted by 0. The present paper and its companion [GKL95] were motivated by a desire to gain a better understanding of the difficulty of finding, in a given d-dimensional convex body C, a j-simplex that is *largest* (of maximum j-measure). The case of a general C is discussed in [GKL95], while the present paper concentrates on the case in which C is a d-cube. Since simplices and cubes are among the most familiar of geometric objects, it seems fair to claim that the problem of finding a largest j-simplex in a given d-cube is a basic problem in computational convexity. However, as we shall see, the special case in which $j = d$ is equivalent to the Hadamard maximum determinant problem, and even the "easy" subcase in which $j = d \equiv 3 \pmod 4$ subsumes the famous problem on the existence of Hadamard matrices. The case of general j and d is equivalent to the problem of constructing D-optimal weighing designs for spring balances. Hence truly definitive results are not to be expected here. However, our geometric approach does yield some new insights and a number of new problems and conjectures.

For use in later sections, Section 1 collects some basic results concerning largest simplices and some formulas expressing simplex volumes in terms of determinants. It also contains some special determinant computations that are needed later. Sections 2–3 concentrate on the case of full-dimensional simplices in a cube (the case $j = d$). Section 2 focuses on the relationship of largest d-simplices to the Hadamard determinant problem, while Section 3 is concerned with parts of the more general question: "How may a bound or a largest d-simplex be situated in a d-cube?" Section 4 deals with pairs (j, d) such that among the largest j-simplices in a d-cube, there is one that is regular and has its centroid at the center of the cube. (Such simplices are called *centrally regular*.) Sections 5–7 contain our principal new results on largest (or conjectured largest) simplices in cubes for cases in which such simplices are not centrally regular. In addition to suggesting directions for further research, Section 8 explains the relationship of largest simplices to D-optimal weighing designs for chemical balances and spring balances.

A few of our proofs are based on results that are not proved until later sections. That is because the organization of the paper has been dictated more by its potential usefulness as a survey than by the logical dependencies among its results.

1. SIMPLEX VOLUMES AND DETERMINANTS

The following definitions are used frequently in later sections. When S is a j-simplex in a convex body C and W is a (possibly empty) set of vertices of S, we say that S is *W-largest* in C if $\mathrm{vol}(S) \geqslant \mathrm{vol}(S')$ for each j-simplex S' in C whose vertex set contains W. If $\mathrm{vol}(S) \geqslant \mathrm{vol}(S')$ (resp. $\mathrm{vol}(S) > \mathrm{vol}(S')$) whenever S' is a j-simplex in C such that each point of W is a vertex of S' and S' is obtained from S by moving a single vertex of S to a new position in C, then S is said to be *W-stable* (resp. *W-rigid*) in C. And S is *W-bound* to C if each vertex of S that is not in W is an extreme point of C. When W is a singleton $\{w\}$, we write *w-largest*, *w-stable*, etc., and when $W = \emptyset$ we write simply *largest*, *stable*, etc. Note that W-largest implies W-stable and W-rigid implies W-stable.

The problem of finding a largest (or stable or rigid) j-simplex S in a d-polytope P consists of two parts, both of which may be difficult when the polytope has many vertices: (a) (the search problem) finding S in the first place, (b) (the verification problem) verifying that S has the desired property. For the very special case in which $j = d$ and the property of interest is that of being stable or rigid (but not that of being largest), there are fast verification algorithms based on linear programming (see 4.3. of [GKL95]). However, it is conjectured in [GKL95] that when j and d are permitted to vary, it is in all other cases $\mathbb{NP}$-hard to decide, for a bound j-simplex in a general d-polytope P that is given as an intersection of halfspaces, whether S is stable in P, rigid in P, or largest in P. The papers [BGKV90, GK92, GK93, GKL95] contain $\mathbb{NP}$-hardness results that tend to support this conjecture or to show the difficulty of determining the volume of a largest j-simplex in a general d-polytope. The d-polytopes used in these hardness proofs are not cubes, but they are often parallellotopes or are formed from parallelotopes in a simple manner. Except for a few special sorts of pairs (j, d) that are discussed in the present paper, we do not expect the computational complexity to be much better when the d-polytope is in fact a d-cube. The present paper focuses on those special sorts of pairs. In this enterprise, an essential role is played by the following four results, which are respectively 2.2, 2.3, 2.4, and 2.6 of [GKL95]. (See [Sh94] for a relative of Theorem 1.1.)

1.1. THEOREM. *Among the W-largest j-simplices in a given body C, there is at least one that is W-bound to C.*

1.2. THEOREM. *If w is a point of a body C and S is a w-stable j-simplex in C, then at least one vertex of S other than w is an extreme point of C.*

1.3. THEOREM. *If S is a stable j-simplex in a body C, then at least two vertices of S are extreme points of C.*

1.4. THEOREM. *Let $v_0, \dots, v_j$ denote the vertices of a W-stable j-simplex S in a given body C. With $r < j$, suppose that*

$W \subset \{v_0, \dots, v_r\}$,

each of the points $v_0, \dots, v_r$ which does not belong to W is an extreme point of C,

none of the points $v_{r+1}, \dots, v_j$ is an extreme point of C.

Then for some i with $r < i \leqslant j$, it is true that each segment in C that crosses v_i is parallel to the affine hull of $\{v_0, \dots, v_r\}$.

Applying Theorem 1.4 to the case in which C is the cube $[0, 1]^d$, we obtain the following consequence.

1.5. COROLLARY. *Suppose that $v_0, v_1, \dots, v_j$ are the vertices of a stable j-simplex in the d-cube $[0, 1]^d$, where v_0 is the origin 0 and $v_1, \dots, v_r$ are also vertices of the cube but (with $r < j$) $v_{r+1}, \dots, v_j$ are not vertices of the cube. Then at least one of the standard basis vectors $e_1, \dots, e_n$ is a linear combination of $v_1, \dots, v_r$.*

Proof. Use Theorem 1.4 in conjunction with the fact that for each nonextreme point p of the cube $[0, 1]^d$ there exists a standard basis vector e_k and there exists $\varepsilon > 0$ such that the segment $[p - \varepsilon e_k, p + \varepsilon e_k]$ is contained in the cube. ∎

The following well-known facts about simplex volumes are used here without specific reference or are referred to as "standard formulas."

- If v is a vertex of a j-simplex S, F is the facet ($(j-1)$-face) of S that misses v, and δ is the distance from v to the affine hull $\mathrm{aff}(F)$ of F, then $\mathrm{vol}(S) = \delta \, \mathrm{vol}(F)/j$.
- If S is a d-simplex in $\mathbb{R}^d$ and A is the $(d+1) \times d$ matrix whose rows list the coordinates of the vertices of S, then $(d!)\mathrm{vol}(S) = |\det(M)|$, where M is the $(d+1) \times (d+1)$ matrix formed from A by appending a column of 1's. If the origin is a vertex of S, then $(d!)\mathrm{vol}(S) = |\det(A_0)|$ where A_0 is formed from A by discarding A's zero row.

• The circumradius and the volume of a regular j-simplex of edge-length λ are respectively equal to

$$\lambda\sqrt{\frac{j}{2(j+1)}}$$

and

$$\frac{\sqrt{j+1}}{j!}\left(\frac{\lambda}{\sqrt{2}}\right)^j.$$

Hence the volume of a regular j-simplex of circumradius ρ is equal to

$$\frac{(j+1)^{(j+1)/2}}{j!j^{j/2}}\rho^j.$$

We also use the fact, proved by Fejes Tóth [Fe64] and Slepian [Sl69], that among the j-simplices contained in a given j-ball, only the regular ones are largest. (Concerning "extreme simplices," there are related but more complicated results due to Slepian [Sl69] and Ali [Al70]. They are not needed here, but may turn out to be useful for future studies extending the present one.)

In addition to the above standard results concerning simplex volumes, we rely heavily on the following result, which expresses the volume of a suitably located simplex in terms of the determinant of the *Gram matrix* formed by the inner products of the vertices of the simplex (see [Bl53, GKL95, 1.5]). (Other formulas expressing simplex volumes in terms of determinants can be found in [GK94] and its references.)

1.6. THEOREM. *Suppose that S is a j-simplex in $\mathbb{R}^d$ with $0 \in \operatorname{aff}(S)$, and A is the $(j+1) \times d$ matrix whose rows list the coordinates of the vertices of S. Then*

$$(j!)^2\operatorname{vol}^2(S) = \det(J + AA^T),$$

where J is the $(j+1) \times (j+1)$ matrix whose entries are all 1. If the origin is a vertex of S then

$$(j!)^2\operatorname{vol}^2(S) = \det(A_0 A_0^T),$$

where A_0 is formed from A by discarding A's zero row.

Among the largest j-simplices in the d-cube $[0, 1]^d$, there is always one that is bound and has one vertex at the origin. Hence finding the maximum volume of a j-simplex in this cube amounts to determining $G(j, d)$, which we define as the maximum of $\det(AA^T)$ as A ranges over all $j \times d$ (0, 1) matrices.

Special cases of the following determinant computations are used in later sections.

1.7. LEMMA. *If A is an $n \times n$ matrix in which each row sum is σ, the square of the norm of each row is ξ, and the inner product of any two distinct rows is η, then*

$$|\det(A)| = |\sigma|(\xi - \eta)^{(n-1)/2}.$$

Proof. For any two distinct row vectors v and w,

$$(v - w) \cdot (v - w) = (v \cdot v) + (w \cdot w) - 2(v \cdot w) = 2(\xi - \eta).$$

Hence the row vectors are the vertices of a regular $(n-1)$-simplex S of edge length $\sqrt{2(\xi - \eta)}$, and by the assumption about row sums these vertices all lie in the hyperplane of $\mathbb{R}^n$ consisting of all points for which the sum of the coordinates is σ. The distance from the origin to this hyperplane is $|\sigma|/\sqrt{n}$, so if T denotes the n-simplex obtained from S by adding the origin as a new vertex, then

$$\mathrm{vol}(T) = \frac{1}{n}\frac{\sigma}{\sqrt{n}}\mathrm{vol}(S).$$

The stated conclusion now follows from the facts that $|\det(A)| = n!\mathrm{vol}(T)$ and

$$\mathrm{vol}(S) = \frac{\sqrt{n}}{(n-1)!}\left(\frac{\sqrt{2(\xi - \eta)}}{\sqrt{2}}\right)^{n-1}.$$

■

1.8. LEMMA. *Let $\varphi_n(\alpha, \beta)$ denote the determinant of the $n \times n$ matrix $M_n(\alpha, \beta)$ whose diagonal entries are all α and off-diagonal entries are all β. Then*

$$|\varphi_n(\alpha, \beta)| = |\alpha + (n-1)\beta||\alpha - \beta|^{n-1}.$$

Proof. Apply the previous lemma with $\sigma = \alpha + (n-1)\beta$, $\xi = \alpha^2 + (n-1)\beta^2$, and $\eta = 2\alpha\beta + (n-2)\beta^2$. ■

1.9. LEMMA. *Suppose that* $\alpha + (r-1)\beta = \mu \neq 0$, *that* C *is an* $r \times s$ *matrix each of whose column sums is equal to* σ, *and that*

$$M = \begin{bmatrix} M_r(\alpha, \beta) & C \\ \tau \cdots \tau & \\ \cdots & M_s(\xi, \eta) \\ \tau \cdots \tau & \end{bmatrix}.$$

Then with $\varepsilon = \sigma\tau/\mu$,

$$|\det(M)| = |\varphi_r(\alpha, \beta)\varphi_s(\xi - \varepsilon, \eta - \varepsilon)|.$$

Proof. The sum of the first r rows of M is the vector $(\mu, \dots, \mu, \sigma, \dots, \sigma)$ with r μ's and s σ's. If $\mu \neq 0$ then subtracting τ/μ times this vector from each of the last s rows of M produces a matrix whose upper left $r \times r$ submatrix is $M_r(\alpha, \beta)$, whose lower left $s \times r$ submatrix is zero, and whose lower right $s \times s$ submatrix is $M_s(\xi - \varepsilon, \eta - \varepsilon)$. ■

Now let I_n denote the $n \times n$ identity matrix, J_n the $n \times n$ matrix whose entries are all 1, and (for $1 \leqslant l \leqslant n$) I_l the $n \times n$ matrix whose entries are all 0 except that its last l diagonal entries are all 1. The following consequence of Lemmas 1.8 and 1.9 is relevant to several results in Sections 6–7, where matrices of the form $k(I_n + J_n) + I_l$ are associated with n-simplices, which, for certain values of d, are the largest n-simplices in Q_d that we have been able to find.

1.10. COROLLARY. $|\det(k(I_n + J_n))| = k^n(n+1)$ *and* $|\det(k(I_n + J_n) + I_l)| = k^n(l+2)((l+n-1)k - l)$.

2. LARGEST d-SIMPLICES IN d-CUBES: THE HADAMARD MAXIMUM DETERMINANT PROBLEM

As a matter of taste, and because of contacts with the companion study [GKL95], many of our results are phrased in terms of maximizing vol(S) over the class of all j-simplices S in a given d-cube, or over certain subclasses of such simplices. The results could equally well be phrased in terms of maximizing certain determinants and are in fact often approached by means of determinants. However, in many cases the geometric formulation seems more natural and interesting. Our main effort is devoted to maximizing vol(S) over *all* j-simplices in the cube $Q_d = [0, 1]^d$. Because of the fact that there is always a largest j-simplex that is bound to Q_d (see 1.1), and because of the symmetries of Q_d, attention may be restricted to j-simplices that are 0-bound to Q_d. In view of Theorem 1.6, the maximization problem is then equivalent to that of maximizing $\det(AA^T)$ over all $j \times j$ (0, 1) matrices A. As is explained in Section 8.I, this amounts to constructing D-optimal weighing designs for spring balances.

Another important problem is that of maximizing the volume of a 0-bound j-simplex in the d-cube $[-1, 1]^d$. Here the condition that the origin 0 should be one of the vertices is a real restriction. In view of Theorem 1.6, the problem becomes that of maximizing $\det(AA^T)$ over all $j \times j$ (± 1) matrices A. As is explained in Section 8.I, this problem amounts to that of constructing D-optimal weighing designs for chemical balances. Section 8.I contains a fairly complete list of references concerning this problem, which has been much more thoroughly studied than the one for spring balances.

In discussing d-cubes, it is often efficient to use a standard form such as the unit d-cube $Q_d = [0, 1]^d$ or the 0-centered d-cube $[-1, 1]^d$. For our present purposes, the two forms have roughly equal claims to convenience. However, to standardize our discussion, we have chosen to frame most of it in terms of Q_d.

By a *corner j-simplex* in a cube we mean a j-simplex whose vertex set consists of a vertex v of the cube along with the j other vertices of the cube that are adjacent (joined by an edge of the cube) to v. From a standard formula it is clear that in Q_d, the volume of each corner j-simplex is $1/j!$ and the volume of any bound j-simplex is an integral multiple of $1/j!$. Hence we take $j!$ as a sort of normalizing factor for the volume of a j-simplex in Q_d, and we define $\rho_{j,d}$ as $j!$ times the volume of a largest j-simplex in Q_d. Since the case $j = d$ is of special interest, $\rho_{d,d}$ is denoted simply by ρ_d. As we shall see, the precise numerical value of ρ_d is known for infinitely many values of d, but it is also unknown for infinitely many d, the smallest being 14.

Results in this section and in Sections 4–5 are expressed explicitly in terms of $\rho_{j,d}$ or ρ_d, but in later sections it is more convenient to express the results in terms of $G(j, d)$, the maximum of $\det(AA^T)$ as A ranges over all $j \times d$ (0, 1) matrices. It follows from Theorem 1.6 that $\rho_{j,d} = \sqrt{G(j, d)}$.

For simplices of dimension lower than that of the containing cube, we do not know of any strong relationship between the problem of maximizing the volume of a simplex in a given cube and that of maximizing the volume of a center-bound simplex in a given cube. However, Theorem 2.1 below shows that in the full-dimensional case, the two problems are equivalent in the sense that a complete solution of either one (for all dimensions of the cube) would imply a complete solution of the other. Finding a largest d-simplex in the cube Q_d is equivalent to finding a largest 0-bound $(d+1)$-simplex in the cube $[-1, 1]^{d+1}$.

There is nothing essentially new about the following theorem (cf. [Wi46, Mo46, Co63, Co65, HW78, GK95]), but the form stated here is especially suitable for our geometric purposes.

2.1. THEOREM. *For each dimension $d \geqslant 1$, the following are all correct descriptions of the volume ratio ρ_d:*

ρ_d is $d!$ times the volume of a largest d-simplex in the d-cube $[0, 1]^d$;
ρ_d is $(d+1)!/2^d$ times the volume of a 0-largest $(d+1)$-simplex in the $(d+1)$-cube $[-1, 1]^{d+1}$;
ρ_d is the maximum of the determinants of the $d \times d$ $(0, 1)$ matrices;
$\rho_d = \alpha_{d+1}/2^d$, where α_n denotes the maximum of the determinants of the $n \times n$ (± 1) matrices.

Proof. The first statement merely repeats the definition of ρ_d. To justify the third statement, use a standard determinantal formula for volume in conjunction with the fact that there is in Q_d a largest d-simplex that has one vertex at the origin.

There is an obvious affine transformation of Q_d onto the cube $[-1, 1]^d$, and it multiplies d-measures by a factor of 2^d. Hence ρ_d is equal to $d!/2^d$ times the volume of a largest d-simplex in the d-cube $[-1, 1]^d$. To justify the second description of ρ_d, use this fact in conjunction with two applications of a standard determinantal formula, first in $[-1, 1]^d$ with no restriction on positions of vertices, and then in $[-1, 1]^{d+1}$, restricting one vertex to be at the origin and using the fact that in this $(d+1)$-cube there is a 0-largest $(d+1)$-simplex that has the point $(1, 1, \ldots, 1)$ as one of its vertices.

To justify the fourth description of ρ_d, use a standard determinantal formula without restricting the position of a vertex, and then note that among the matrices relevant to α_n there is one whose first column consists entirely of 1's. ■

In preparation for later results, we want to describe more explicitly the important matrix-to-simplex and simplex-to-simplex correspondences that are implicit in the above proof.

Suppose first that A is a $(d+1) \times (d+1)$ (± 1) matrix of nonzero determinant. Then the rows of A provide the $d+1$ nonzero vertices of a 0-bound $(d+1)$-simplex in the $(d+1)$-cube $[-1, 1]^{d+1}$, and the volume of this simplex is $|\det(A)|/(d+1)!$. Now, for each column of A that starts with -1, replace that column by its negative. This preserves the absolute value of the determinant and hence also the volume of the corresponding $(d+1)$-simplex, which now has the point $(1, 1, \ldots, 1)$ as one of its vertices. Next, for each row of A that starts with -1, replace that row by its negative. The absolute value of the determinant is preserved, and now both the first row and the first column of the matrix consist of 1's. When the first column is discarded, the remaining $d+1$ row vectors form the vertices of a d-simplex S in the d-cube $[-1, 1]^d$. This d-simplex is of volume $|\det(A)/d!|$ and one of its vertices is the point $(1, 1, \ldots, 1) \in [-1, 1]^d$. Finally, in the last d columns of the matrix, replace all 1's by 0 and all -1's by 1. This is the result of an affine transformation of the cube $[-1, 1]^d$ onto the cube $Q_d = [0, 1]^d$, carrying the vertex $(1, 1, \ldots, 1)$ of the former onto the vertex $(0, 0, \ldots, 0)$ of the latter. The transformation multiplies d-measures by 2^{-d}, and the lower right $d \times d$ submatrix M of A now provides the d nonzero vertices of a d-simplex in Q_d that has the origin as one of its vertices. The volume of this simplex is equal to $|\det(M)|/d!$, and

$$|\det(M)| = \frac{1}{2^d d!} \det(A).$$

Thus we have passed from a $(d+1)$-simplex with vertex at the origin in the $(d+1)$-cube $[-1, 1]^{d+1}$ to a d-simplex with vertex at the origin in the d-cube $Q_d = [0, 1]^d$, and the volume of the d-simplex is $d/2^d$ times the volume of the $(d+1)$-simplex from which it arose. Further, it is clear that all but the very first step is reversible, so that from an arbitrary d-simplex with vertex 0 in Q_d we obtain a $(d+1)$-simplex with vertices 0 and $(1, 1, \ldots, 1)$ in $[-1, 1]^{d+1}$.

This is an appropriate place to mention a notational distinction between the present paper and its companion [GKL95]. The dimension of the ambient space is usually denoted by n in [GKL95], while here it is denoted by d. There are two reasons for this. Some of the main results in [GKL95] concern the computational complexity of finding a largest j-simplex in a given polytope, for the case of polytopes of varying dimension. The dimension is there called n because that is traditional in computational geometry and because it agrees with the notation in an earlier related paper [GK93]. In the present paper, however, questions of computational complexity are not considered explicitly, and much of the focus is on specific (rather than varying) values of the ambient dimension. Hence we have chosen to denote that dimension by d to reserve n for speaking, as is traditional, of $n \times n$ matrices. As can be seen from Theorem 2.1, finding a largest d-simplex in a d-cube is equivalent to maximizing the determinant of a $d \times d$ $(0, 1)$ matrix and is also equivalent to maximizing the determinant of a $(d + 1) \times (d + 1)$ (± 1) matrix. Hence for a given value of d, the n of primary interest may be either d or $d + 1$, depending on which simplex-to-matrix correspondence one has in mind.

The *Hadamard maximum determinant problem* is the problem of determining as many as possible of the above numbers α_n or, equivalently, of the volume ratios ρ_d. It is called this because of the 1893 theorem of Hadamard [Ha93] asserting that $\alpha_n^2 \leqslant n^n$, with equality if and only if there exists an $n \times n$ (± 1) matrix whose columns (equivalently, whose rows) are pairwise orthogonal. Such matrices are called *Hadamard matrices* (hereafter, *H-matrices*), and the problem of determining the n for which they exist (the *H-numbers*) is known as the *Hadamard matrix problem*. Thus the Hadamard maximum determinant problem subsumes the Hadamard matrix problem. Sylvester [Sy67] showed that each power of 2 is an H-number. Hadamard showed that, aside from 1 and 2, each H-number is divisible by 4, and he showed that 12 and 20 are H-numbers. Later authors greatly extended the list of H-numbers, and Paley [Pa33] conjectured that every multiple of 4 is an H-number. (This conjecture has often been attributed to [Ha93], but it does not appear there in any explicit way.)

All the known constructions of H-matrices depend on special number-theoretic, combinatorial, or algebraic properties of n in addition to its being a multiple of 4, and there are infinitely many multiples of 4 that are not known to be H-numbers. We refer to the surveys of Geramita and Seberry [GS79], Agaian [Ag85], Wallis [Wa88], and Seberry and Yamada [SY92] for the extensive results and literature on the H-matrix problem, to Sawade [Sa85], Yamada [Ya89], and Miyamoto [Mi91] for some of the most recent constructions of H-matrices, and to Hedayat and Wallis [HW78] and Agaian [Ag85] for the many applications of H-matrices.

Now we summarize the known results on the Hadamard maximum determinant problem. (For other surveys of this problem, see [BC72, Sm87].) Results in the original papers are stated in terms of α_n. However, we restate several of them here in terms of the volume ratio ρ_d because that is more natural and more useful for our present geometric approach. Let us begin with a theorem of Williamson [Wi46]. (See [Co94] for related results.)

2.2. THEOREM.

$$\alpha_3 = 4, \qquad \alpha_4 = 16, \qquad \alpha_5 = 48, \qquad \alpha_6 = 160, \qquad \alpha_7 = 576.$$

Let two matrices be called "equivalent" if each can be obtained from the other, or from the other's transpose, by a sequence of operations each of which consists of interchanging two rows or columns or multiplying a row or column by -1. *Then for the values of* n *specified below, each* $n \times n$ (± 1) *matrix of determinant* α_n $(= 2^{n-1}\rho_{n-1})$ *is equivalent to the following matrix* W_n:

$$W_3 = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \\ 1 & 1 & -1 \end{pmatrix}, \qquad W_4 = \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \\ 1 & -1 & 1 & -1 \end{pmatrix},$$

$$W_5 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 \\ 1 & -1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 & -1 \\ 1 & -1 & -1 & -1 & 1 \end{pmatrix}$$

$$W_6 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & 1 & 1 & -1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & -1 & -1 & 1 \end{pmatrix},$$

$$W_7 = \begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & 1 & -1 & -1 & 1 \\ 1 & 1 & 1 & -1 & -1 & -1 & -1 \\ 1 & -1 & -1 & -1 & 1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 & -1 & -1 & 1 \end{pmatrix}.$$

Note that the matrices W_3–W_6 are symmetric, but W_7 is not.

2.3. THEOREM.

$$\rho_2 = 1, \qquad \rho_3 = 2, \qquad \rho_4 = 3, \qquad \rho_5 = 5, \qquad \rho_6 = 9.$$

For $2 \leqslant d \leqslant 5$, *each largest* d-*simplex in* Q^d *is equivalent, with respect to the isometries of* Q_d, *to the* d-*simplex whose vertex set consists of the origin* *along with the row vectors of the matrix M_d below. Each largest 6-simplex in Q_6 is similarly equivalent to the 6-simplex provided by the origin along with the row vectors or the column vectors of M_6:*

$$M_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \qquad M_3 = \begin{pmatrix} 0 & 1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}, \qquad M_4 = \begin{pmatrix} 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \end{pmatrix},$$

$$M_5 = \begin{pmatrix} 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}, \qquad M_6 = \begin{pmatrix} 1 & 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}.$$

Proof. This is a consequence of Williamson's theorem in conjunction with the correspondences described in the paragraph following the proof of Theorem 2.1. ■

Note that if S and T are 6-simplices whose respective vertex sets are given by the origin along with the rows or the columns of M_6, then S and T are not equivalent under the symmetry group of Q_6. Indeed, one edge of S is of length $\sqrt{5}$, while no edge length of T exceeds 2.

Our statements of the remaining results in this section are all in terms of ρ_d. They are translations (based on Theorem 2.1) of the original results, which in each case concerned the values of determinants of (± 1) matrices. For example, Hadamard's result [Ha93] may be stated in the following form, where the geometric conditions for equality are explained in Section 4.

2.4. THEOREM. *For each d,*

$$\rho_d^2 \leqslant (d+1)\left(\frac{d+1}{4}\right)^d.$$

When $d > 1$, equality implies that $d \equiv 3 \pmod 4$. Equality is equivalent to each of the following conditions:

(i) *$d+1$ is an H-number; i.e., there exists a $(d+1) \times (d+1)$*

Hadamard matrix;

(ii) *in the d-cube* $Q_d = [0, 1]^d$ *there is a largest d-simplex that is regular.*

As far as we know, Colucci [Co26] was the first to sharpen Hadamard's inequality for the case in which $4 \nmid d + 1$. Next was Barba [Ba33]. He provided a heuristic argument for the following result, which was later proved rigorously (and independently) by Ehlich [Eh64a].

2.5. THEOREM. *For all even d,*

$$\rho_d^2 \leqslant (2d + 1)\left(\frac{d}{4}\right)^d.$$

Equality never holds when $d \equiv 2 \pmod 4$, *and when* $4 | d$ *equality implies that* $2d + 1$ *is a perfect square.*

For the case in which $d \equiv 2 \pmod 4$, the upper bound of Theorem 2.5 has been sharpened by Ehlich [Eh64b] and Smith [Sm87], but it seems that no cases of equality are associated with those bounds either. However, Smith's approach by means of hyperbolic space is interesting in itself.

Aside from the case in which $d \equiv 3 \pmod 4$ (the case of α_n when $4 | n$), the most progress in determining ρ_d has been made when $d \equiv 1 \pmod 4$. The following result is due to Ehlich [Eh64a] and Wojitas [Wo64].

2.6. THEOREM. *If* $d \equiv 1 \pmod 4$ *and* $d \neq 1$, *then*

$$\rho_d^2 \leqslant d^2\left(\frac{d-1}{4}\right)^{d-1}.$$

Equality implies that $2d$ *is the sum of two squares.*

The following result summarizes the work of many authors.

2.7. THEOREM. *The equality*

$$\rho_d^2 = (d + 1)\left(\frac{d+1}{4}\right)^d$$

holds for infinitely many $d \equiv 3 \pmod 4$, *including all such* $d < 427$. *The equality*

$$\rho_d^2 = (2d + 1)\left(\frac{d}{4}\right)^d$$

holds for $d \in \{4, 12, 24, 40\}$, *and infinitely many larger* $d \equiv 0 \pmod 4$ *and the equality*

$$\rho_d^2 = d^2\left(\frac{d-1}{4}\right)^{d-1}$$

holds for $d \in \{5, 9, 13, 17, 25, 29, 3741, 45, 61, 65, 73, 81, 85, 89, 97, 101\}$ *and infinitely larger* $d \equiv 1 \pmod 4$. *Also,*

$$\rho_2 = 1, \qquad \rho_6 = 9, \qquad \rho_8 = 56, \qquad \rho_{10} = 320, \qquad \rho_{13} = 9{,}477,$$
$$\rho_{16} = 327{,}680, \qquad \rho_{20} = 56{,}640{,}625.$$

The first equality corresponds to the existence of Hadamard matrices of various orders, and the many contributors are too numerous to mention here. For these we refer again to the surveys of [HW78, GS79, Ag85, Wa88, SY92] mentioned earlier, and we refer also to [Sa85] for the fact that $n = 428$ is the smallest multiple of 4 for which the existence of an $n \times n$ Hadamard matrix is unknown.

The constructions that establish the second equality are due to Williamson [Wi46], Raghavarao [Ra59], Ehlich and Zeller [EZ62], Wojitas [Wo64], Trung [Tr82], and Neubauer and Radcliffe [NR96]. They cover all dimensions d such that $4 \leqslant d < 60$, $4|d$, and $2d + 1$ is a perfect square.

The constructions that establish the third equality are due to Ehlich [Eh64a], Yang [Ya66a,b,68,69,76], Cohn [Co89,92], and Neubauer and Radcliffe [NR96]. They cover all dimensions d such that $1 < d < 109$, $d \equiv 1 \pmod 4$, and $2d$ is the sum of two squares. All of these authors use circulant matrices in an elegant manner suggested by Ehlich, and Cohn's approach yields more general information about the forms of matrices that can attain equality in this case.

For $d < 30$, all but 11 values of ρ_d are covered by the cases of equality mentioned in Theorems 2.4–2.7. Among those eleven, ρ_8, ρ_{10}, ρ_{13}, ρ_{16}, and ρ_{20} have been determined by a mixture of mathematics and computer search [EZ62, EH64a, Mi74a, GK80b, MK82, CKM87], but it appears that the precise values of ρ_{14}, ρ_{18}, ρ_{21}, ρ_{22}, ρ_{26}, and ρ_{28} are still unknown. The integers 14, 18, 22, and 26 belong to the especially difficult case of $d \equiv 2 \pmod 4$. Since 42 is not the sum of two squares, ρ_{21} is less than the upper bound provided by Theorem 2.4, and since 57 is not a perfect square, ρ_{28} is less than the upper bound provided by Theorem 2.5. Cohn [Co89] conjectured that $\rho_{14} = 25{,}515$. Smith [Sm87] made the same conjecture, and his computations led also to conjectured values (and associated matrices) for ρ_{18}, ρ_{21}, and ρ_{22}. However, his conjectured value for ρ_{21} is significantly less than the value (stated in Theorem 2.7) that was proved in [CKM87]. (These results and conjectures were all phrased originally in terms of α_{d+1} rather than ρ_d.)

Brenner and Cummings [BC72] have references to several lower bounds on α_n that are known to hold for all n. The one that we use here is due to Clements and Lindström [CL65]. When combined with Hadamard's inequality and stated in terms of ρ_{d-1}, it can be written in the following form.

2.8. THEOREM. *For all d,*

$$\frac{1}{2}\left(1 - \frac{\log(4/3)}{\log d}\right) d \log d < \log(2^{d-1}\rho_{d-1}) \leqslant \frac{1}{2} d \log d,$$

with equality on the right if and only if d is an H-number.

For a strengthening of the lower bound, see [Sc70].

3. MOVING A BOUND d-SIMPLEX IN A d-CUBE

This section considers a few aspects of the following general question: How may a bound or a largest d-simplex be situated in a d-cube? In particular, it demonstrates the severe limitations of the attempt to find a largest simplex by starting with a single bound simplex and then trying to steadily increase the volume by moving one vertex at a time along an edge of the cube.

For a bound simplex S in a d-polytope P, we define a *k-move* as the act of replacing S by a bound simplex S' (of the same dimension) that is obtained by moving a single vertex v of S to a different vertex of P that shares a k-face with v. The move is called *good* if $\mathrm{vol}(S) > \mathrm{vol}(S')$ and *fair* if $\mathrm{vol}(S) \geqslant \mathrm{vol}(S')$. The simplex S is called *k-stable* if it does not admit any good k-move and *k-rigid* if it does not admit any fair k-move. When $k = d$, these notions are the same as the stability and rigidity defined in Section 1. However, the present section focuses on the case in which $k = 1$ and P is Q_d. In this case, a 1-move of a bound simplex S amounts to changing a single coordinate of a vertex of S from 0 to 1 or vice versa. (See [GKL95] for some properties of 1-moves of simplices in general convex polytopes.)

The following remarks explain, among other things, why several fair moves may be necessary before a good move can be made.

3.1. THEOREM. *Suppose that $d \geqslant 2$, that S is a bound d-simplex in Q_d, and that k facets of S are contained in facets of Q_d. Then $k \leqslant d$, with $k = d$ if and only if S is a corner simplex. No 1-move of S can reduce k by more than 1. When $k \geqslant d - 1$, S does not admit a good 1-move.*

Proof. No facet of Q_d contains more than one facet of S, and since $d \geqslant 2$ it cannot happen that two opposite facets of Q_d contain facets of S. Hence $k \leqslant d$, and there is a vertex v of S (and of Q_d) that is incident to all of the k facets of S that are contained in facets of Q_d. Obviously $k = d$ if S is a corner simplex. Conversely, if $k = d$ then each edge of S incident to v is contained in the intersection of the d facets of Q_d incident to v, whence each such edge is an edge of Q_d and S must be a corner simplex.

To prove the next assertion, note that for each edge $[v, v']$ of Q_d, there is a unique facet of Q_d that contains v but not v'. It follows that when a new d-simplex S' is produced by moving a vertex v of S to the other end of an edge incident to v, there will still be at least $k - 1$ facets of Q_d that contain facets of S.

(The preceding two paragraphs use only the fact that the d-polytope Q_d is *simple* in the sense that each of its vertices is incident to precisely d edges. The remainder of the proof makes additional use of the special structure of Q_d.)

Now suppose that $k \geqslant d - 1$, and assume without loss of generality that the origin is incident to each of the k facets of S that lies in a facet of Q_d. Let M denote the $(d + 1) \times d$ matrix whose first row is 0 and whose later rows list the coordinates of the d nonzero vertices of S, and let M' be formed by discarding the first row of M. Then $\mathrm{vol}(S) = |\det(M')|/d!$. Since $k \geqslant d - 1$, there are at least $d - 1$ columns of M' that consist of all 0's except for a single 1. No two of these 1's share a row, for if they did then M' would have two identical columns and hence zero determinant. Thus by permuting rows we may assume that M' has the form that for simplicity is shown below only for $d = 5$ (it will be clear that the ensuing argument actually applies to all d):

$$M' = \begin{pmatrix} 1 & 0 & 0 & 0 & \alpha \\ 0 & 1 & 0 & 0 & \beta \\ 0 & 0 & 1 & 0 & \gamma \\ 0 & 0 & 0 & 1 & \delta \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

We want to show that the volume of the simplex S cannot be increased by changing a single entry of M from 0 to 1 or vice versa. Let us first consider the entries of M'. Any change of a diagonal entry changes $\det(M')$ to 0, and if a nondiagonal entry not in the last row is changed then the changed M' can be carried by column operations to the identity matrix. If the change involves the last row of M', we may assume by symmetry that it consists of changing the first entry in that row from 0 to 1. But then $\alpha = 0$, for otherwise the changed M' would have two identical rows and hence determinant zero. Now an upper triangular matrix with determinant 1 is obtained from the changed M' by subtracting the first row from the last one.

The discussion up to this point shows that if the volume of S can be increased by a 1-move, then that move replaces the origin as a vertex of S by a vertex of Q_d that has a single coordinate equal to 1. Hence the relevant entry of the matrix M is in its first row, and by symmetry it may be assumed to lie in the first or last column of M. Let N denote the matrix obtained from M by appending a column of 1's. Then $\mathrm{vol}(S) = |\det(N)|/d!$, and we are concerned with the effect on $|\det(N)|$ of the indicated change in M. The two possibilities for the changed N are as follows:

$$N_1 = \begin{pmatrix} 1 & 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 & \alpha \\ 1 & 0 & 1 & 0 & 0 & \beta \\ 1 & 0 & 0 & 1 & 0 & \gamma \\ 1 & 0 & 0 & 0 & 1 & \delta \\ 1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \qquad N_2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 & \alpha \\ 1 & 0 & 1 & 0 & 0 & \beta \\ 1 & 0 & 0 & 1 & 0 & \gamma \\ 1 & 0 & 0 & 0 & 1 & \delta \\ 1 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

Straightforward row and column operations show that $|\det(N_1)| = |\alpha|$ and $\det(N_2) = 0$, thus completing the proof. ■

For a bound 3-simplex in Q_3, the vertex set of S is completely determined (up to isometries of the cube) by specifying the number j of facets of S that are contained in facets of Q_3. The four possibilities are as follows:

$$\begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}.$$

The indicated tetrahedra S have k equal to 3, 2, 1, and 0, respectively, and they are of volume $1/6$, $1/6$, $1/6$, and $1/3$, respectively. Here S admits a good 1-move if and only if $k = 1$, hence is 1-stable if and only if $k \neq 1$. The conditions that $k = 0$, that S is 1-rigid, that S is rigid, and that S is largest are in this case equivalent. Of course the situation becomes much more complicated as the dimension increases, but at least the following aspect of the 3-dimensional situation persists.

3.2. THEOREM. *With $d \geqslant 3$, suppose that S is a bound d-simplex in Q_d and some facet F of S is contained in a facet G of Q_d. Then S admits a sequence of d or fewer fair 1-moves in which the last move is a good one.*

Proof. Let G' denote the facet of Q_d opposite G, and for each vertex u of G let u' denote the vertex of G' that is adjacent to u in Q_d. There are d vertices of S—say $v_0, \ldots, v_{d-1}$—in G and the remaining vertex v_d of S belongs to G'. The d vertices determine a $(d-1)$-simplex F, and when $d \geqslant 3$ there is at least one $(d-2)$-face of this simplex—say $\operatorname{conv}\{v_0, \ldots, v_{d-2}\}$—that fails to be contained in a $(d-1)$-face of the $(d-1)$-cube G. Let H denote the hyperplane that contains the set

$$\{v_0, \ldots, v_{d-2}, v'_0, \ldots, v'_{d-2}\}.$$

If v_d is strictly separated from v_{d-1} by H, then

$$\operatorname{dist}(v'_{d-1}, \operatorname{aff}\{v_0, \ldots, v_{d-2}, v_d\}) > \operatorname{dist}(v_{d-1}, \operatorname{aff}\{v_0, \ldots, v_{d-2}, v_d\})$$

and hence moving v_{d-1} to v'_{d-1} is a good move for S.

Now suppose that v_d is not strictly separated from v_{d-1} by H, and let w be any vertex of G' that is separated from v_{d-1} by H. Since G' is a $(d-1)$-cube, G' contains a path from v_d to w that is formed from $d-1$ or fewer edges of G'. Each move of v_d along one of those edges is fair, because it preserves the distance of the moving vertex from the hyperplane $\operatorname{aff}(F)$ $(= \operatorname{aff}(G))$. Hence there is a sequence of $d-1$ or fewer fair 1-moves that reduces the situation to the one in the preceding paragraph, and then a good 1-move is possible. ∎

As an illustration of increasing complexity as the dimension d increases, we mention the two 5-simplices whose vertices are given by the rows of the following matrices:

$$\begin{pmatrix} 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}, \qquad \begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{pmatrix}.$$

The first simplex has three facets contained in facets of Q_5, and it admits a good 1-move. (Moving $(1, 0, 0, 0, 0)$ to $(1, 1, 0, 0, 0)$ increases the determinant from 1 to 2.) The second simplex has no facet contained in a facet of Q_5. As the following result shows, it is rigid but not largest.

3.3. LEMMA. *Suppose that v is a vertex of Q_d and S is a d-simplex whose vertex set consists of the vertex of Q_d opposite to v and the d vertices of Q_d adjacent to v. Then S is rigid when $d \geqslant 3$ but is largest if and only if $d \leqslant 4$.*

Proof. We assume without loss of generality that v is the origin, so the vertices v_i of S are given by $v_i = e_i$ (a standard basis vector) for $1 \leqslant i \leqslant d$ and $v_0 = \Sigma_{i=1}^{d} e_i$. One facet of S is the $(d-1)$-simplex $\operatorname{conv}\{v_1, \ldots, v_d\}$. The hyperplane containing F consists of all points for which the sum of coordinates is 1, and the parallel hyperplane through v_0 consists of all points for which the sum of coordinates is d. Since v_0 is the only vertex of Q_d on the latter hyperplane, any move of v_0 to another vertex of Q_d on v_0's side of H reduces the distance to H and hence results in a simplex of smaller volume. The only vertex of Q_d on the other side of H is the origin, and it is closer to H than v_0 is. Hence v_0 is not involved in any fair move for S.

Because of the symmetry involving the remaining facets of S, it suffices to consider just one of them—say $\operatorname{conv}\{v_0, \ldots, v_{d-1}\}$. Let H denote the hyperplane that contains this facet. Then the parallel hyperplane through v_d consists of all points $(\xi_1, \ldots, \xi_d)$ such that

$$-(d-2)\xi_d + \sum_{i=1}^{d-1} \xi_i = -(d-2),$$

hence intersects the cube only at v_d. It follows that moving v_d to any point of the cube on v_d's side of H would reduce the distance to H and thus reduce the volume of the simplex. The same is true of moving v_d to any point of the cube on the other side of H, and hence the simplex S is rigid.

To complete the proof, we show that for $d \geqslant 5$, S is not a largest d-simplex in Q_d. An easy computation shows that the volume of S is $(d-1)/(d!)$. Checking against the values of ρ_d given in Section 2, we see that S is a largest d-simplex in Q_d when $d \in \{3, 4\}$ but not when $d \in \{5, 6\}$. It remains only to show that S is not largest when $d \geqslant 7$, and that follows easily from the lower bound in Theorem 2.9. ■

The following conditions on a d-polytope P are satisfied by some polytopes and fail for others. They are all relevant to the attempt to find a largest d-simplex in P by starting with some d-simplex, attempting to improve it by moving one vertex at a time, then if necessary trying another starting d-simplex, etc.

M_1: If a bound d-simplex S in P is not largest, then S admits a sequence of successive fair 1-moves leading to a largest d-simplex.

M_2: If a bound d-simplex S in P admits a fair 1-move, then it admits a sequence of successive fair 1-moves ending in a good 1-move.

M_3: If a bound d-simplex S in P is largest, it is rigid.

While P always admits a largest d-simplex that is bound, the following property is relevant to the task of finding *all* largest d-simplices:

B: Each largest d-simplex in P is bound.

For general polytopes, (generalizations of) the properties M_1–M_3 and B are discussed in [GKL95]. Here we focus on the special case of cubes, and we start by using the above lemmas to decide when the d-cube has property M_1.

3.4. THEOREM. *It is precisely when $d \leqslant 4$ that the d-cube has the following property*:

> *Starting from an arbitrary bound d-simplex, there is a sequence of fair 1-moves that leads to a largest d-simplex.*

For $d \geqslant 5$, this property fails even if arbitrary fair moves are permitted.

Proof. The case $d \geqslant 5$ is settled by Lemma 3.3. The case $d = 2$ is trivial, because all bound triangles in Q_2 are largest. The case $d = 3$ follows from Theorem 3.2, and also from the representation of bound tetrahedra given after the proof of Theorem 3.1.

It remains only to show that Q_4 has property M_1, and in view of Theorem 3.2 it suffices to consider a bound 4-simplex S such that no facet of Q_4 contains more than three vertices of S. This implies that for each pair of two opposite facets of Q_4, one of them contains three vertices of S and the other contains two vertices of S. At this point, we originally completed the proof by means of a purely mathematical argument that took about a page and involved (of course!) a division into several cases. However, we report instead on the results of a later computational experiment that served the same purpose.

We generated, in Q_4, all 4-tuples of nonzero vertices, these vertices to be taken along with the origin as those of a bound 4-simplex in Q_4. For each 4-tuple we used the coordinates of the respective vertices to form the rows of a 4×4 matrix. Each matrix was tested to see whether at least one of its column sums was equal to 4 or was less than or equal to 1. A matrix in which a column sum is 0 corresponds to a 4-simplex having four vertices in addition to the origin on the same facet of Q_4, so those matrices were discarded. A matrix in which a column sum is 1 or 4 corresponds to a 4-simplex in which some facet is contained in a facet of Q_4, and by Lemma 3.2 each such simplex admits a sequence of 4 or fewer fair 1-moves terminating in a good 1-move. Hence it was sufficient to test the remaining matrices. It turned out that each of them either had determinant 0 (hence did not correspond to a 4-simplex) or admitted a change of a single entry (from 0 to 1 or vice versa) that increased the value of the determinant. That was sufficient to complete the proof. ■

Let $\mathscr{S}_i$ denote the collection of al bound 4-simplices of volume $i/24$ in Q_4. Since $\rho_4 = 3$, the members of $\mathscr{S}_3$ are the largest 4-simplices in Q_4. From the above discussion it follows that each member of $\mathscr{S}_1$ can be transformed into a member of $\mathscr{S}_3$ by using at most five fair 1-moves, while each member of $\mathscr{S}_2$ requires only a single fair 1-move to be turned into a largest simplex.

3.5. THEOREM. *When $d + 1$ is an H-number, and also when d is 4 or 5, each largest d-simplex in Q_d is bound and rigid. For each d such that $7 \leqslant d \leqslant 30$ and the value of ρ_d is known (this excludes the cases of $d \in \{14, 18, 21, 22, 26\}$), there is in Q_d a largest d-simplex that is bound and 1-rigid, but we do not know whether this is true of all largest d-simplices in Q_d. When d is 2 or 6, no largest d-simplex in Q_d is 1-rigid. When $d = 10$, Q_d contains unbound largest d-simplices, largest d-simplices that are bound but not 1-rigid, and largest d-simplices that are bound and 1-rigid.*

Proof. Suppose first that $d + 1$ is an H-number, whence each largest d-simplex S in Q_d is (by 4.2–4.3 in the next section) bound and regular. If d vertices of S are fixed, they form an equilateral set of edge length $\sqrt{d+1}/2$, and there are only two points of $\mathbb{R}^d$ that can be added to these d vertices to produce the vertex set of a regular d-simplex. Each of those points is at distance $(d + 1)/2\sqrt{d}$ from the hyperplane determined by the d vertices, and the distance between the two points is $(d + 1)/\sqrt{d}$. To complete the proof for this case, note that this exceeds the diameter of Q_d. (For a stronger rigidity result when $d + 1$ is an H-number, see Theorem 4.6.)

The statement of 3.5 is obvious for $d = 2$. When d is 4 or 5, each largest d-simplex in Q_d is equivalent, with respect to the cube's symmetries, to the one given in Theorem 2.3. It is easy to check the rigidity of these by an argument similar to the one used in proving Lemma 3.3, or by direct computation. For $d = 6$, computation was used to discover that if the entry in position $(1, 4)$ of the matrix W_7 (of Theorem 2.2) is replaced by its negative, then the value (576) of the determinant is unchanged; in fact, the submatrix of W_7 that remains after the first row and the fourth column of W_7 is deleted has determinant 0. Now let M denote the matrix formed by the last six columns of W_7 and let S denote the 6-simplex whose ith vertex is given by the $(i + 1)$th row of M. Then $v_0 = (1, 1, 1, 1, 1, 1)$, and the edge of $[-1, 1]^6$ joining v_0 to the vertex $(1, 1, -1, 1, 1, 1)$ is parallel to the facet determined by the remaining vertices of S. Hence S is not even 1-rigid in the cube in question. The same phenomenon can of course be observed with the simplices provided by the origin along with the rows or columns of the matrix M_6 of Theorem 2.3. However, it turns out that the origin is the only vertex that can be moved without decreasing the volume, so the representation provided by Theorem 2.4 is not computationally the most convenient one.

The remaining observations in Theorem 3.5 result from applying the "toggle test" to various $n \times n$ (± 1) matrices M_n (with $n = d + 1$) known to have determinant α_n. (These matrices were obtained from the papers or from the authors mentioned in the preceding section.) The toggle test consists of comparing the determinant of the original matrix M_n to the determinants of the n^2 matrices obtained by changing the sign of a single entry of M_n. If any of the toggled matrices has the same absolute determinant as M_n, then Q_d contains a largest d-simplex that is not 1-rigid and hence also contains a largest d-simplex that is not bound. If all of the toggled matrices have smaller absolute determinant than the original, then Q_d contains a largest d-simplex that is 1-rigid.

The case $d = 10$ is especially interesting. We tested five 11×11 (± 1) matrices (associated with [EZ62, Eh64b, GK80b]) of the same maximum determinant 327,680. For one of them, the toggle test led to rigidity (i.e., each toggle reduced the determinant); but each of the remaining four choices of M_{11} has four entries whose signs could be switched without changing the determinant. ■

We conjecture that if Q_d contains a largest d-simplex that is not rigid, then d is of the form $4k + 2$.

3.6. THEOREM. *The d-cube has a property* M_2 *when d is* 3 *or* 4 *but not when d is* 2, 6, *or* 10.

Proof. For an arbitrary d-polytope P, Theorem 3.1 of [GKL95] tells us that $M_2 \Rightarrow M_3$. When $d \in \{2, 6, 10\}$, Q_d lacks M_3 by Theorem 3.5 and hence also lacks M_2. When $d \in \{3, 4\}$, Q_d has M_1 by Theorem 3.4 and M_3 by Theorem 3.5, and the conjunction of these two properties implies M_2. ■

4. CENTRAL REGULARITY OF LARGEST j-SIMPLICES IN d-CUBES

A j-simplex is *regular* if the $\binom{j+1}{2}$ pairs of its vertices all determine the same distance. This section, and, in part, Sections 5–6, are concerned with some of the ways in which a largest j-simplex in a d-cube can be regular. The following three possibilities are considered:

- $j \in R_d^c$, meaning that in Q_d there is a largest j-simplex that is regular and whose centroid is at the center $(\frac{1}{2}, \dots, \frac{1}{2})$ of Q_d;
- $j \in R_d^\forall$, meaning that every largest j-simplex in Q_d is regular;
- $j \in R_d^\exists$, meaning that at least one bound largest j-simplex in Q_d is regular.

We show below (Corollary 4.3) that $R_d^c \subset R_d^\forall$, and since there is always a largest j-simplex that is bound (Theorem 1.1), it is clear that $R_d^\forall \subset R_d^\exists$. Results in Section 5 show that for some values of d, R_d^c can be a proper subset of $R_d^\forall$. However, we do not know whether $R_d^\forall$ can be a proper subset of $R_d^\exists$ and we do not know whether, when $j \in R_d^\exists$, there is necessarily a largest j-simplex in Q_d that is both bound and regular.

The present section focuses on the set R_d^c, and our results on the sets $R_d^\forall \setminus R_d^c$ and $R_d^\exists \setminus R_d^c$ are incorporated in Sections 5–6 as part of the more general effort of finding largest j-simplices in d-cubes.

For each $d \geqslant 2$, the d-cube $\{-1, 1\}^d$ contains an equilateral set of d points with distance $\sqrt{8}$. However, this set is linearly dependent only when $d = 2$. The following lemma shows that for linearly dependent equilateral subsets of $\{-1, 1\}^d$, each of the quantities *cardinality* and *distance* is determined by the other.

4.1. LEMMA. *With* $j \geqslant 1$, *suppose that* $j + 1$ *linearly dependent points of* $\{-1, 1\}^d$ *form an equilateral set with distance* δ. *Then* $\delta = \sqrt{2d(j+1)/j}$, $d(j+1)$ *is divisible by* $4j$, *and the origin is the centroid of the j-simplex that is the convex hull of the points.*

Proof. Let the points be $p_0, \ldots, p_j$. For each pair (i, r) with $i \neq r$, it is true that $(p_i - p_r)\cdot(p_i - p_r) = \delta^2$ and hence the value of $p_i \cdot p_r$ is a constant $\gamma = (2d - \delta^2)/2$. By hypothesis, there are constants γ_i, not all 0, such that $\sum_{i=0}^{j}\gamma_i p_i = 0$. Hence for each index i,

$$\gamma_i(p_i \cdot p_i) + \sum_{i \neq r} \gamma_i(p_i \cdot p_r) = 0.$$

With $\sigma = \sum_{i=0}^{j}\gamma_i$, it follows that $\gamma_i d + (\sigma - \gamma_i)\gamma = 0$, whence $\gamma_i(d - \gamma) = -\sigma\gamma$, and summing on i yields $\sigma(d - \gamma) = -(j + 1)\sigma\gamma$. If $\sigma = 0$, then (take $\gamma_i \neq 0$) $\gamma = n$, which implies $\delta = 0$. Therefore $\sigma \neq 0$, so it follows that $\gamma j = -n$ and hence $\delta = \sqrt{2d(j + 1)/j}$. The distance δ is equal to $2\sqrt{c}$, where c is the number of coordinates that change in the passage from p_0 to p_1 and is also the number of coordinates that change in the passage from p_1 to p_2. If b denotes the number of coordinates in which the first change is cancelled by the second, then $2c - 2b$ is the number of coordinates in which p_0 and p_2 differ. But this is also equal to c, so we have $8b = 4c = \delta^2 = 2d(j + 1)/j$ and $d(j + 1) = 4bj$.

It is easy to verify that for any equilateral set $X = \{p_0, \ldots, p_j\}$ in $\mathbb{R}^d$, the centroid $(1/(j + 1))\sum_{i=0}^{j} p_i$ is the only point of the affine hull aff(X) that is equidistant from all points of X. In the present situation, our assumption that the set X is linearly dependent implies that its affine hull is the same as its linear hull, so $0 \in$ aff(X) and 0 must be the centroid of X. (In fact, the proof could have begun with this observation, in which case some of the details could have been slightly simplified.) ■

Theorem 2.4 (a geometric form of Hadamard's theorem) is concerned with d-simplices in Q_d. Here is an extension to j-simplices in Q_d.

4.2. THEOREM. *For $1 \leqslant j \leqslant d$,*

$$\rho_{j,d}^2 \leqslant (j + 1)\left(\frac{j + 1}{4}\right)^j\left(\frac{d}{j}\right)^j.$$

In this inequality, equality implies that $4j|d(j + 1)$, and equality is equivalent to each of the following conditions:

(i) $j \in R_d^c$;

(ii) *in the d-cube $Q_d = [0, 1]^d$ there is an equilateral set of $j + 1$ points with distance $\sqrt{d(j + 1)/2j}$;*

(iii) *in* Q_d *there is a bound regular* j*-simplex whose centroid is the center of* Q_d;

(iv) *a set of cardinality* d *can be covered by* j *sets* $B_1, \ldots, B_j$ *such that* $|B_i| = d(j+1)/2j$ *for each* i *and* $|B_i \cap B_r| = d(j+1)/4j$ *for each* $i \neq r$.

Further, the center of the cube Q_d *is the centroid of each set of the sort described in* (ii) *and of each simplex of the sort described in* (iii).

Proof. By definition,

$$\rho_{j,d} = j!\big(\text{volume of largest } j\text{-simplex in } [0,1]^d\big).$$

Therefore

$$\begin{aligned}
\left(\frac{2^j}{j!}\right)\rho_{j,d} &= \big(\text{volume of largest } j\text{-simplex in } [-1,1]^d\big)\\
&\leqslant \big(\text{volume of largest } j\text{-simplex in a } d\text{-ball of radius } \sqrt{d}\,\big)\\
&= \big(\text{volume of largest } j\text{-simplex in a } j\text{-ball of radius } \sqrt{d}\,\big)\\
&= \big(\text{volume of regular } j\text{-simplex inscribed in a } j\text{-ball of radius } \sqrt{d}\,\big)\\
&= \left(\sqrt{\frac{d(j+1)}{j}}\right)^j \big(\text{volume of regular } j\text{-simplex inscribed in a } j\text{-ball of radius } 1\big)\\
&= \left(\sqrt{\frac{d(j+1)}{2j}}\right)^j \left(\frac{\sqrt{j+1}}{j!}\right)\left(\frac{1}{\sqrt{2}}\right)^j,
\end{aligned}$$

whence the stated inequality follows.

To justify the second equality in the above sequence, note that for a j-simplex in a d-ball, the affine hull of the simplex intersects the d-ball in a j-ball, and the radius of the j-ball is a maximum if and only if the j-ball is concentric with the d-ball. For the third equality, use the fact [Fe64, Sl69] that among all the j-simplices inscribed in a given j-ball, it is precisely the regular ones that are of maximum volume. These facts also make it possible to work backward and to show that equality is indeed characterized by each of the first two stated criteria. To produce the sets described in (iii), start with a largest j-simplex that has the origin as one vertex, and let the sets $B_1, \ldots, B_j$ consist of the coordinate positions in which the remaining vertices have coordinate 1. Note finally that from the sets in (iii) it is a routine matter to produce the points in (i). ■

4.3. COROLLARY. *If $j \in R_d^c$ then each largest j-simplex in a d-cube is regular, bound, and rigid, and has its centroid at the center of the cube. Hence $R_d^c \subset R_d^\vee$.*

Proof. Suppose that $j \in R_d^c$. Then the statements about regularity, about being bound, and about the centroid are immediate from the preceding theorem. Now if a largest j-simplex fails to be rigid, there are two largest j-simplices that have j vertices in common and are both regular. But that is impossible when each of the j-simplices has the cube's center as its centroid. ■

When S is a simplex in a centrally symmetric convex body C, we say that S is *central* in C provided that the centroid of S is at the center of C. If, in addition, the simplex S is regular, we say that S is *centrally regular* in C. It follows with the aid of Theorem 1.3 that if a centrally regular j-simplex S in a d-cube Q is a largest j-simplex in Q, then it is also a largest j-simplex in the ball that circumscribes Q; from this it follows that S is bound to Q. In the next section we encounter (for $j = 2$ and $j = 4$) circumstances in which a j-simplex in a cube can be bound and regular but not central. However, we do not know whether, when a largest j-simplex S in a cube happens to be regular, S must be bound to the cube.

Let $h(n)$ denote the maximum of the cardinalities of the orthogonal subsets of $\{-1, 1\}^n$. An easy argument of Hadamard [Ha93] shows that $h(n) = 1$ when n is odd, $h(n) = 2$ when n is divisible by 2 but not by 4, and $3 \leqslant h(n) \leqslant n$ when n is a multiple of 4. The H-numbers are those for which $h(n) = n$. In explaining the relationship of H-numbers and H-matrices to regular simplices, the following remark is useful.

4.4. LEMMA. *$h(d+1) \geqslant k$ if and only if some k points of $\{-1, 1\}^d$ form an equilateral set with distance $\sqrt{2d+2}$.*

Proof. For "only if," let X be an orthogonal set of k points in $\{-1, 1\}^{d+1}$, and assume without loss of generality that each point of X has 1 as its first coordinate. For each $x \in X$, discard the first coordinate to form the point $x' \in \{-1, 1\}^d$. Then $x' \cdot y' = -1$ for any two distinct points x and y of X, whence

$$(x' - y') \cdot (x' - y') = (x' \cdot x') + (y' \cdot y') - 2(x', y') = 2d - 2(-1)$$

and $\sqrt{2d + 2}$ is the distance between x' and y'.

For "if," simply reverse the preceding construction, noting that if an equilateral set in $\{-1, 1\}^d$ has distance $\sqrt{2d + 2}$, then each pair of its points has inner product -1 and hence orthogonality results when a new coordinate 1 is appended to each point. ■

In particular, $h(d + 1) = d + 1$ if and only if some $d + 1$ points of $\{-1, 1\}^d$ form an equilateral set of distance $\sqrt{2d + 2}$), and this is equivalent to saying that some $d + 1$ points of $\{0, 1\}^d$ form an equilateral set of distance $\sqrt{(d + 1)/2}$. That explains the condition for equality in Theorem 2.4.

The relationship between H-matrices and regular simplices has been discussed by many authors, including Barrau [Ba07], Barba [Ba33], Coxeter [Co33], Gruner [Gr39], Hadwiger [Ha56], Dedò [De68], Grigorév [Gr80], Dolnikov [Do87], and Pichugov [Pi88]. See the last two references and the brief discussion in Section 8.C for the role that this relationship plays in the geometry of Minkowski spaces.

4.5. THEOREM. *For each dimension d, the following three conditions are equivalent*:

(i) $d \in R_d^{\forall}$; *i.e., in a d-cube, every largest d-simplex is regular*;
(ii) *the vertex set of a d-cube contains an equilateral set of $d + 1$ points*;
(iii) *there exists an H-matrix of order $d + 1$.*

Proof. By Theorem 1.1, there is a largest d-simplex all of whose vertices are vertices of the cube. Hence (i) implies (ii).

If the set $\{-1, 1\}^d$ contains an equilateral set of $d + 1$ points, then by Lemma 4.1 the distance between any two of these points is $\sqrt{d + 1}$. It then follows from Lemma 4.3 that $h(d + 1) = d + 1$; i.e., there exists an H-matrix of order $d + 1$. Hence (ii) implies (iii).

Now suppose that there exists an H-matrix of order $d + 1$. Then there exists such a matrix A whose first column consists entirely of 1's. Remove A's first column, and regard each row of the remaining matrix as a point of $\{-1, 1\}^d$. These $d + 1$ points are the vertices of a regular d-simplex S in the cube $[-1, 1]^d$, and

$$\operatorname{vol}(S) = |\det(A)|/d!.$$

From the fact that equality in Hadamard's inequality is achieved (in the case of real matrices) precisely by the H-matrices, and from the reversibility of the just-mentioned passage from $(d+1) \times (d+1)$ (± 1) matrices to d-simplices with vertices in $\{-1, 1\}^d$, it follows that S is a largest d-simplex in the cube $[-1, 1]^d$. Hence (iii) implies (i). ■

The following observation is due to D. Ljubič.

4.6. THEOREM. *Suppose that $d + 1$ is an H-number. If two largest d-simplices in Q_d have at least $d - 2$ vertices in common, then they coincide.*

Proof. Let $d = 4k - 1$. For each facet F of Q_d, let F' denote the unique facet of Q_d that is disjoint from F. Since each largest d-simplex in Q_d has its centroid at the origin, each such d-simplex must have $2k$ vertices in F and $2k$ vertices in F'. Further, by an application of Theorem 4.2 to $(2k-1)$-simplices in $(4k-2)$-cubes, we see that for each largest d-simplex S in Q_d, the centroids of the $(2k-1)$-simplices $S \cap F$ and $S \cap F'$ must be at the centers of F and F' respectively.

Now suppose that V and W are the vertex sets of two largest d-simplices in Q_d and that

$$|V \cap W \cap F| + |W \cap T \cap F'| \geqslant 4k - 3$$

for each pair F, F'. Then for each such pair, at least one of F or F' must contain at least $2k - 1$ points that are common to V and W. Suppose it is F that does this. Then, since each of the sets $V \cap F$ and $W \cap F$ consists of just $2k$ points and has its centroid at the center of F, it follows that $V \cap F = W \cap F$.

We see from the preceding paragraph that if $V \neq W$ then there is a facet G of Q_d that contains two points (say p and p') that belong to $V \setminus W$. Let H and H' be disjoint facets of Q_d that contain p and p' respectively. Then, on the one hand, $V \cap H \neq W \cap H$ and $V \cap H' \neq W \cap H'$, but, by the general statement about F and F' we must have $V \cap H = W \cap H$ or $V \cap H' = W \cap H'$. The contradiction completes the proof. ■

By condition (ii) of Theorem 4.5, if the subset $\{0, 1\}^d$ of $\mathbb{Z}^d$ contains the vertex set of a regular d-simplex, then $d + 1$ is an H-number and hence (except when $d = 1$) $d \equiv 3 \pmod 4$. It is interesting in this connection to recall the theorem of Schoenberg [Sc37], Pelling [Pe77], and Macdonald [Ma87], which asserts that the integral lattice $\mathbb{Z}^n$ contains the vertex set of a regular d-simplex if and only if d satisfies one of the following conditions:

(i) $d \equiv 3 \pmod 4$;
(ii) $d \equiv 0 \pmod 4$ and $d + 1$ is a perfect square;
(iii) $d \equiv 1 \pmod 4$ and $(d + 1)/2$ is a sum of two squares.

The tool for proving this is the theory of rational equivalence of quadratic forms.

Theorem 4.5 provides a satisfactory answer, modulo the conjecture on the existence of H-matrices, to the question of when $d \in R_d^{\forall}$. We do not have an equally satisfactory answer to the question of when $d \in R_d^{\exists}$. On the one hand, we know of no example in which $R_d^{\exists} \neq R_d^{\forall}$, but, on the other hand, we do not know how to prove even that $d + 1$ is divisible by 4 whenever $d \in R_d^{\exists}$. However, the following two results do show that if $d + 1$ is not divisible by 4 and d is any dimension for which the precise value of the volume ratio ρ_d is currently known, then $d \notin R_d^{\exists}$.

4.7. Lemma. *If S is a stable j-simplex in Q_d and S is regular, then*

$$\operatorname{vol}(S)^2 = \frac{j+1}{(j!)^2}\left(\frac{m}{2}\right)^k$$

for some integer m.

Proof. The volume of a regular j-simplex S of edge length λ is equal to

$$\frac{\sqrt{j+1}}{j!}\left(\frac{\lambda}{\sqrt{2}}\right)^j.$$

If S is stable in Q_d, then by Theorem 1.3 at least two vertices of S are also vertices of Q_d, whence λ^2 is an integer and the stated conclusion follows. ∎

4.8. Theorem. *If any of the following conditions is satisfied, then $d \notin R_d^{\exists}$; that is, no largest d-simplex in a d-cube is regular:*

(i) $d \equiv 0 \pmod 4$ *and equality holds in Theorem* 2.5;
(ii) $d \equiv 1 \pmod 4$ *and equality holds in Theorem* 2.6;
(iii) $d \in \{2, 6, 8, 10, 13, 20\}$.

Proof. If $d \in R_d^{\exists}$ then it follows from Lemma 4.7 that ρ_d^2 is of the form $(d+1)(m/2)^d$ for some integer m. Under (i) this yields

$$(d+1)m^d 2^d = (2d+1)d^d,$$

and under (ii) it yields

$$(d+1)m^d 2^{d-2} = d^2(d-1)^{d-1},$$

both of which are impossible because $d+1$ is relatively prime to each of d, $d-1$, and $2d+1$. Similar divisibility arguments apply in case (iii). ∎

4.9. LEMMA. *If $j \in R_d^c$ then $j \in R_{kd}^c$ for each positive integer k.*

Proof. Let $B_1, \ldots, B_j$ be a system of j sets that covers a set D of cardinality d and satisfies the cardinality requirements in condition (iv) of Theorem 4.2. Let K be a set of cardinality k. Then the set $D \times K$ is of cardinality kd and is covered by the sets $B_i' = B_i \times K$. These sets satisfy (iv)'s cardinality conditions for the pair (j, kd). ∎

4.10. THEOREM. *If $8j+4$ is an H-number, then $4j+1 \in R_{k(8j+2)}^c$ for each positive integer k.*

Proof. Let H_0 be an $(8j+4) \times (8j+4)$ H-matrix whose entries in the first row and the first column are all -1. Permute the columns of H_0 so that the second column is $(-1, \ldots, -1, 1, \ldots, 1)^T$. Then let H be the $(4j+1) \times (8j+2)$ submatrix of H_0 such that $H_{ik} = (H_0)_{i+1,k+2}$.

Visually, we have

$$H_0 = \begin{pmatrix} -1 & -1 & -1 & \cdots & -1 & -1 & \cdots & -1 \\ -1 & -1 & H_{11} & \cdots & H_{1,4j} & H_{1,4j+1} & \cdots & H_{1,8j+2} \\ \vdots & \vdots & \vdots & & & & & \vdots \\ -1 & -1 & H_{4j+1,1} & \cdots & H_{4j+1,4j} & H_{4j+1,4j+1} & \cdots & H_{4j+1,8j+2} \\ -1 & 1 & \pm 1 & & & & & \pm 1 \\ \vdots & \vdots & & & & & & \\ -1 & 1 & \pm 1 & & & & & \pm 1 \end{pmatrix}.$$

Since H_0 is presumed to be an H-matrix, each row of H_0 except the first has $4j+2$ 1's and $4j+2$ -1's. Therefore, each row of H has $4j+2$ 1's and $4j$ -1's. Further, each row shares $2j+1$ 1's with each other row.

Now, let $P = \frac{1}{2}(H + J)$. Then each row of P has $4j + 2$ 1's and $4j$ 0's and each row shares $2j + 1$ 1's with each other row. Hence $PP^T = (2j + 1)(I + J)$, and therefore the rows of P and the origin are the vertices of a regular simplex S in the cube Q_{8j+2}. Further, the centroid of S is the center $(\frac{1}{2}, \dots, \frac{1}{2})$ of the cube. The stated conclusion now follows from Theorem 4.2 and Lemma 4.9. ∎

4.11. LEMMA. *Suppose that S is a bound regular j-simplex in a d-cube C, that the centroid of S is the center of C, and that some i-face F of S is contained in an r-face G of C. If $(j - i)d = (i + 1)j(d - r)$, then $i \in R_r^c$.*

Proof. Since F is a regular j-simplex, it suffices to show that the centroid of F coincides with the center of the r-cube G. Now note that if P is a cube or a regular simplex, E is a proper face of P, and p and e are the centroids of P and E respectively, then e is the unique point of E nearest to p and E is contained in the hyperplane that passes through e orthogonal to the segment $[p, e]$. Hence it suffices in our present situation to show that the centroids of F and of G are equidistant from the center of C.

An easy computation (working with the regular j-simplex that is the convex hull of a standard basis for $\mathbb{R}^{j+1}$) shows that in a regular j-simplex S of edge length λ, the distance between the centroid of S and the centroid of an i-face of S is equal to

$$\frac{\lambda}{\sqrt{2}}\sqrt{\frac{j-i}{(j+1)(i+1)}}.$$

Normalizing the present situation by taking the cube C to be Q_d, we have $\lambda = \sqrt{d(j+1)/2j}$. Since the distance from the center of Q_d to the centroid of an r-face of Q_d is equal to $\sqrt{d-r}/2$, the centroids of F and G are equidistant from the center of C if and only if

$$\frac{\sqrt{d(j+1)/2j}}{\sqrt{2}}\sqrt{\frac{j-i}{(j+1)(i+1)}} = \frac{\sqrt{d-r}}{2}.$$

This reduces to the stated condition that $(j - i)d = (i + 1)j(d - r)$. ∎

4.12. COROLLARY. *The first two statements below are equivalent, they imply the third one, and at least when $d \equiv 3 \pmod 8$ they are equivalent to the third one*:

(i) $d+1$ *is an H-number*;
(ii) $d \in R_d^c$;
(iii) $(d-1)/2 \in R_{d-1}^c$.

Proof. The equivalence of (i) and (ii) follows from 4.2–4.3. That (ii) implies (iii) follows from Lemma 4.11, as can be seen by setting $j = d$, $i = (d-1)/2$, and $r = d - 1$. When $d \equiv 3 \pmod 8$, it follows from Theorem 4.10 that (iii) implies (ii). ∎

We do not know how to prove that (iii) implies (ii) when $d - 3$ is divisible by 4 but not by 8. However, this seems a safe conjecture because a counterexample would require a multiple of 4 that is not an H-number.

We close this section with a few more results on R_d^c.

4.13. THEOREM. *For each k, $3 \in R_{3k}^c$ and $5 \in R_{10k}^c$.*

Proof. In view of Lemma 4.9, it suffices to show that $3 \in R_3^c$ and $5 \in R_{10}^c$. That $3 \in R_3^c$ follows from Theorem 4.2, since 4 is an H-number. To see that $5 \in R_{10}^c$, let A be the 5×10 matrix whose columns are all possible arrangements of three 1's and two 0's; i.e.,

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

The rows of A, along with the origin, form the vertex set of a regular 5-simplex T of edge length $\sqrt{6}$. Since T's centroid is the center $(\frac{1}{2}, \ldots, \frac{1}{2})$ of Q_d, it follows from Theorem 4.2 that T is a largest 5-simplex in Q_{10} and $5 \in R_{10}^{\forall}$. ∎

4.14. THEOREM. *For each pair of positive integers j and k,*

$$2j + 1 \in R^c_{k\binom{2j+1}{j+1}}.$$

Proof. In view of Theorem 4.2, it suffices to exhibit in the $\binom{2j+1}{j+1}$-dimensional unit cube a bound regular $(2j+1)$-simplex whose centroid is the center of the cube. Let A be the $(2j+1) \times \binom{2j+1}{j+1}$ matrix whose columns are all possible arrangements of j zeros and $j+1$ ones. For example, if $j = 2$, then

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}.$$

Letting S be the $(2j+1)$-simplex whose vertices are the origin and the rows of A, we claim that S is both regular and largest in the unit $\binom{2j+1}{j+1}$-dimensional cube.

We show first that S is regular. To enumerate the 1's in the first row, we count the columns whose first entries are 1's. The remaining entries of these columns constitute all possible arrangements of j 0's and j 1's, so there are $\binom{2j}{j}$ such columns. Hence the first row has $\binom{2j}{j}$ 1's, and by symmetry the same is true of all other rows.

Now, we count the columns whose first two entries are 1's. The remaining entries of these columns constitute all possible arrangements of j 0's and $j-1$ 1's, so there are $\binom{2j-1}{j}$ such columns. Hence there are $\binom{2j-1}{j}$ columns in which the first and second rows both have a 1. By symmetry, the same is true of each pair of rows.

By these computations, we have determined that

$$\begin{aligned} AA^T &= \left(\binom{2j}{j} - \binom{2j-1}{j}\right)I + \binom{2j-1}{j}J \\ &= \left(\binom{2j-1}{j-1} + \binom{2j-1}{j} - \binom{2j-1}{j}\right)I + \binom{2j-1}{j}J \\ &= \binom{2j-1}{j-1}I + \binom{2j-1}{j}J \\ &= \binom{2j-1}{j}(I+J). \end{aligned}$$

This demonstrates that S is regular, since $AA^T = p(I+J)$ for some p.

Since each column of A has $j + 1$ ones, the centroid of S is the center $(\frac{1}{2}, \ldots, \frac{1}{2})$ of the cube, and hence S is a largest j-simplex by Theorem 4.2. ∎

The following result, similar in spirit to those of the present section, follows from a result of Jacroux and Notz [JN83] that is stated at the end of Subsection 8I.

4.15. THEOREM. *Suppose that S is a bounded j-simplex in Q_d with one vertex at the origin and A is the corresponding matrix. If*

$$AA^T = (d(j + 1)/4j)(I + J), \qquad \text{if } j \text{ is odd}$$

$$AA^T = (d(j + 2)/4(j + 1))(I + J), \qquad \text{if } j \text{ is even}$$

then S is regular and is a largest j-simplex in Q_d.

When j is even, we can use this result to obtain largest simplices in some cases where bounding sphere arguments do not apply. For instance, when $j = 4$ and $d = 10$, we see that the 4×10 matrix A whose columns consist of all arrangements of $\{1, 1, 0, 0\}$ or $\{1, 1, 1, 0\}$ corresponds to a largest 4-simplex in Q_{10}, for $AA^T = 3(I + J)$. This exemplifies the fact that when we have a j-simplex that satisfies the theorem's condition for odd j, then we may remove one vertex of this simplex to obtain also a largest $(j - 1)$-simplex in Q_d.

5. LARGEST 2- AND 3-SIMPLICES IN d-CUBES

It can happen that R_d^{c} is a proper subset of $j \in R_d^{\forall}$. For example, we show below that

$$2 \in R_d^{\forall} \Leftrightarrow 3 \in R_d^{\forall} \Leftrightarrow 3|d \Leftrightarrow 2 \in R_d^{\exists} \Leftrightarrow 3 \in R_d^{\exists}.$$

However, when $j = 2$, condition (iii) of Theorem 4.2 would require that a set X of cardinality d be covered by two sets of cardinality $3d/4$ whose intersection is of cardinality $3d/8$, thus implying that

$$d = |X| = 2\frac{3d}{4} - \frac{3d}{8} = \frac{9d}{8}.$$

The explanation is that, although the largest triangles in a d-cube are regular whenever $d|3$, when $d \geqslant 3$ they are not coplanar with the cube's center. On the other hand, we saw in Section 4 that when $d|3$ the largest 3-simplices in a d-cube are regular and they have the cube's center as their centroid.

To specify a vertex of Q_d, we often use 0_r to denote a string of r 0's, 1_t to denote a string of t 1's, etc. For example, $1_2 0_3$ denotes the vertex $(1, 1, 0, 0, 0)$ of Q_5. We also use $0 \rightarrow$ to indicate that all coordinates beyond a certain point are 0. For example, $1_2 0 \rightarrow$ denotes $(1, 1, 0, 0, 0)$ when it is clear from context that we are working in Q_5, and for any $d \geqslant 2$, $1_2 0 \rightarrow$ denotes the vertex of Q_d whose first two coordinates are 1 with all remaining coordinates (if there are any) equal to 0.

5.1. THEOREM. *If T is a largest triangle in Q_d with $d \geqslant 3$, then T is bound.*

Proof. By Theorem 1.3, at least two of T's vertices (say v_0 and v_1) are vertices of Q_d. Because of the cube's symmetries, we may assume without loss of generality that $v_0 = 0_d$ (the origin) and $v_1 = 1_r 0 \rightarrow$ with $1 \leqslant r \leqslant d$. If the third vertex v_2 of T is not a cube vertex, it follows from Corollary 1.5 that one of the standard basis vectors is a multiple of v_1, whence $r = 1$. But then, since no point of Q_d is at distance greater than $\sqrt{d-1}$ from the line $\mathbb{R}v_1$, the area of T is at most $\sqrt{d-1}\,/2$. However, that is not the maximum possible, for when $d > 3$ the triangle with vertices 0_d, $1_{d-2}0_2$, and 1_d has area $\sqrt{d-2}\,/\,\sqrt{2}$ and when $d = 3$ the triangle with vertices $(1, 0, 0)$, $(0, 1, 0)$, and $(0, 0, 1)$ has area $\sqrt{3}\,/2$, in each case contradicting the hypothesis that T is of maximum area. ■

5.2. THEOREM. *Suppose that $d = 3m + i$ with $0 \leqslant i < 3$. Then the largest triangles in the cube Q_d are of*

$$\textit{area } \frac{d}{2\sqrt{3}} \left(= \frac{\sqrt{3}\,m}{2} \right) \quad \textit{when } i = 0$$

and

$$\textit{area } \frac{\sqrt{d^2 - 1}}{2\sqrt{3}} \quad \textit{when } i \neq 0.$$

Proof. We may assume that a largest triangle has vertices $v_0 = 0$, $v_1 = 1_r 0 \rightarrow$, and (with $s \leqslant r$ and $t \leqslant d - r$) $v_2 = 1_s 0_{r-s} 1_t 0 \rightarrow$. The square of the triangle's area is equal to four times the quantity

$$\|v_1\|^2 + \|v_2\|^2 - (v_1 \cdot v_2)^2 = r(s+t) - s^2.$$

We are interested in maximizing this quantity, and since it increases with t we may assume that $t = d - r$, thus obtaining

$$\|v_1\|^2 + \|v_2\|^2 - (v_1 \cdot v_2)^2 = \frac{1}{3}d^2 - \frac{1}{12}g(d, r, s)$$

with

$$g(d, r, s) = (3r - d)^2 + 3(2s - r)^2.$$

Hence for each fixed d, we are interested in minimizing $g(d, r, s)$. With $d = 3m + i$, it is easy to verify the following:

when $i = 0$,
$g(d, r, s) \geqslant 0$, with equality if and only if $r = 2m$ and $s = m$;
when $i = 1$,
$g(d, r, s) \geqslant 4$, with equality if and only if $r = 2m$ and $s = m$;
when $i = 2$,
$g(d, r, s) \geqslant 4$, with equality if and only if $r = 2m + 1$ and $s = m$.

When expressed in terms of d, these results lead to the areas stated in Theorem 5.2 for the largest triangles in Q_d. ■

By a *nicely regular j-simplex* in Q_d, we mean a regular j-simplex S that satisfies the following conditions:

$j \geqslant 2$;
one vertex v_0 of S is at the origin 0_d;
the remaining vertices $v_1, \ldots, v_j$ of S are also vertices of Q_d.

Under these conditions, there exists an integer w such that each of the vertices $v_1, \ldots, v_j$, has precisely w coordinates equal to 1. This w is called the *weight* of S. It is immediate from the definitions that $w > 1$ and $d \geqslant 3$.

5.3. THEOREM. *Suppose that $d = 3m + i$ with $0 \leqslant i < 3$. Then the nicely regular triangles of weight $2m$ (and those equivalent to them under the cube's symmetries) are precisely the largest regular triangles among the regular triangles that are bound to the cube. These triangles are of*

$$\text{edge length } \sqrt{2m} \quad \text{and} \quad \text{area } \sqrt{3}\,m/2,$$

and when $i = 0$ they are also precisely the largest triangles in Q_d. However, when $i \neq 0$ they are not even the largest regular triangles in Q_d.

Proof. Note, in the proof of the preceding theorem, that the largest triangles determined there are regular exactly when $i = 0$, $r = 2m$, and $s = m$. That proves the stated result when $i = 0$.

When $i = 2$ and $m = 0$, the result is obvious, for of course there are equilateral triangles with positive area inside the unit square Q_2. For the case in which $i \neq 0$ and $m \geqslant 1$, it suffices to exhibit in Q_d an equilateral triangle in Q_d whose edge length exceeds $\sqrt{2m}$. In fact, the triangle with vertices

$$\begin{pmatrix} v_1 = & 0_{3m+j}, & & & & & & & \\ v_2 = & 1_{m-1} & 1_{m-1} & 0_{m-1} & 1 & 1 & (2-\sqrt{2}) & 0 & 0_{j-1}, \\ v_3 = & 1_{m-1} & 0_{m-1} & 1_{m-1} & 0 & (2-\sqrt{2}) & 1 & 1 & 0_{j-1} \end{pmatrix}$$

is equilateral and its edge length is $\sqrt{2m + 6 - 4\sqrt{2}} > \sqrt{2m}$. ■

5.4. COROLLARY. *For each d:*

$$2 \notin R_d^c;$$

$$3 | d \Leftrightarrow 2 \in R_d^{\forall} \Leftrightarrow 2 \in R_d^{\exists}.$$

5.5. THEOREM. *Suppose that $d = 3m + i$ with $0 \leqslant i < 3$. Then the nicely regular tetrahedra of weight $2m$ (and those equivalent to them under the cube's symmetries) are precisely the largest regular tetrahedra that are* *bound. These tetrahedra are of*

$$\textit{edge length } \sqrt{2m} \qquad \textit{and} \qquad \textit{volume } \sqrt{m^3}/3,$$

and when $i = 0$ they are precisely the largest tetrahedra in Q_d. However, when $i \neq 0$ they are not even the largest regular tetrahedra in Q_d.

Proof. Suppose first that $i = 0$. By Theorem 5.2, each largest triangle in Q_d is equivalent to a nicely regular triangle of weight $2m$—say with vertices $v_0 = 0_{3m}$, $v_1 = 1_{2m}0_m$, and $v_2 = 1_m0_m1_m$. To these three vertices we can add a fourth vertex $v_3 = 0_m1_{2m}$ to form a regular tetrahedron with edge length $\sqrt{2m}$ and volume $\sqrt{m^3}/3$. Since, among tetrahedra of a given surface area, it is precisely the regular ones that have maximum volume (cf. [Fe64, p. 283]) it follows from the results on largest triangles that the largest tetrahedra in Q_{3m} are precisely those equivalent to the one whose vertices we have just described. We conclude also (again by using the results on largest triangles) that these are the largest regular tetrahedra whose vertices are all among those of the cube. However, when $i \neq 0$ they are not the largest tetrahedra in the cube because a larger one can be produced by leaving v_0 at the origin and choosing the remaining three vertices as follows:

$$\begin{array}{llllll}
v_0 = & 0_{3m+i} & & & & \\
v_1 = & 1_m & 1_m & 1 & 0_m & 0_{i-1} \\
v_2 = & 1_m & 0_m & 1 & 1_m & 0_{i-1} \\
v_3 = & 0_m & 1_m & 1 & 1_m & 0_{i-1}.
\end{array}$$

With the aid of Theorem 1.6 we see that the volume of this tetrahedron is $\sqrt{4m^3 + 3m^2}/6$, which exceeds $\sqrt{m^3}/3$ for $m > 0$.

Also, when $i \neq 0$ and $m \geqslant 1$, we may exhibit a regular tetrahedron in Q_d whose edge length exceeds $\sqrt{2m}$ and three of whose vertices are not vertices of Q_d. Consider the vertices

$$\left(\begin{array}{lllllllll}
v_1 = & 0_{3m+i}, & & & & & & & \\
v_2 = & 1_{m-1} & 1_{m-1} & 0_{m-1} & 1 & 1 & 1/5 & 0 & 0_{i-1}, \\
v_3 = & 1_{m-1} & 0_{m-1} & 1_{m-1} & 0 & \alpha_1 & 1 & \alpha_2 & 0_{i-1}, \\
v_4 = & 0_{m-1} & 1_{m-1} & 1_{m-1} & \beta_1 & \beta_2 & \beta_3 & 1 & 0_{i-1}
\end{array}\right),$$

where

$$\alpha_1 = \frac{41}{50} = .82000000$$

$$\alpha_2 = \frac{\sqrt{919}}{50} \approx .60630026$$

$$\beta_1 = \frac{8155 + 250\sqrt{919} + 209\sqrt{-57 + 100\sqrt{919}}}{29060} \approx .93366833$$

$$\beta_2 = \frac{1861 - 16\sqrt{919} - 25\sqrt{-57 + 100\sqrt{919}}}{2906} \approx .00429631$$

$$\beta_3 = \frac{14381 - 450\sqrt{919} + 205\sqrt{-57 + 100\sqrt{919}}}{29060} \approx .41017677.$$

These vertices form a regular tetrahedron in Q_d of edge length $\sqrt{2m + \frac{1}{25}} > \sqrt{2m}$. ■

5.6. COROLLARY. *For each d,*

$$3|d \Leftrightarrow 3 \in R_d^c \Leftrightarrow 3 \in R_d^\forall \Leftrightarrow 3 \in R_d^\exists.$$

We conclude this section with a computation of the actual volume of a largest 3-simplex in Q_d. A result equivalent to this is stated but not proved in Mood's paper [Mo46].

5.7. THEOREM. *If $d = 3n + i$ with $i \in \{0, 1, 2\}$, then a largest 3-simplex in Q_d has volume $\sqrt{n^{3-i}(n+1)^i}/3$.*

Proof. Let T be a bound largest tetrahedron in Q_d, with one vertex at the origin 0. The other vertices will have all coordinates in $\{0, 1\}$, so we may arrange them in a $3 \times n$ matrix A of 0's and 1's. Furthermore, we may permute the columns of A so that they appear in blocks:

$$A = \begin{pmatrix} \underbrace{\begin{matrix} 0\cdots 0 \\ 0\cdots 0 \\ 1\cdots 1 \end{matrix}}_{k_1} & \underbrace{\begin{matrix} 0\cdots 0 \\ 1\cdots 1 \\ 0\cdots 0 \end{matrix}}_{k_2} & \underbrace{\begin{matrix} 0\cdots 0 \\ 1\cdots 1 \\ 1\cdots 1 \end{matrix}}_{k_3} & \underbrace{\begin{matrix} 1\cdots 1 \\ 0\cdots 0 \\ 0\cdots 0 \end{matrix}}_{k_4} & \underbrace{\begin{matrix} 1\cdots 1 \\ 0\cdots 0 \\ 1\cdots 1 \end{matrix}}_{k_5} & \underbrace{\begin{matrix} 1\cdots 1 \\ 1\cdots 1 \\ 0\cdots 0 \end{matrix}}_{k_6} & \underbrace{\begin{matrix} 1\cdots 1 \\ 1\cdots 1 \\ 1\cdots 1 \end{matrix}}_{k_7} \end{pmatrix}$$

where k_i is the number of columns in the ith block.

We then note that $\mathrm{vol}(T) = \sqrt{\det(AA^T)}\,/6$, and so it is sufficient to maximize

$$\det(AA^T)$$
$$= \det\begin{pmatrix} k_4 + k_5 + k_6 + k_7 & k_6 + k_7 & k_5 + k_7 \\ k_6 + k_7 & k_2 + k_3 + k_6 + k_7 & k_3 + k_7 \\ k_5 + k_7 & k_3 + k_7 & k_1 + k_3 + k_5 + k_7 \end{pmatrix}.$$

Let us denote this latter determinant by $\psi(k_1, k_2, k_3, k_4, k_5, k_6, k_7)$.

We now examine the effect on ψ of manipulating the columns of A. Our basic strategy is to shrink some blocks of A and inflate others so that the dimensions of A are unchanged. Of course, we want to ensure that none of these manipulations decreases $\det(AA^T)$.

Our first task is to shrink blocks 1, 2, and 4 and inflate blocks 3, 5, and 6 in such a way as to increase $\det(AA^T)$. Suppose that k_1, k_2, and k_4 are all positive. Then we may shrink blocks 1, 2, and 4 by one column each and expand blocks 3, 5, and 6 by one column each. If A_1 denotes the newly obtained matrix, then

$$\det(A_1 A_1^T) - \det(AA^T)$$
$$= \psi(k_1 - 1, k_2 - 1, k_3 + 1, k_4 - 1, k_5 + 1, k_6 + 1, k_7)$$
$$- \psi(k_1, k_2, k_3, k_4, k_5, k_6, k_7)$$
$$= k_1k_2 + k_1k_3 + k_2k_3 + k_1k_4 + k_2k_4 + k_1k_5 + k_3k_5 + k_4k_5 + k_2k_6$$
$$+ k_3k_6 + k_4k_6 + k_5k_6.$$

The expression on the right is composed of nonnegative terms and hence the entire expression is nonnegative. It follows that, without decreasing the value of $\psi(k_1, k_2, k_3, k_4, k_5, k_6, k_7)$, we may repeatedly shrink blocks 1, 2, and 4 until one of them is empty. We may therefore suppose without loss of generality that $k_4 = 0$.

Now, suppose that k_1 and k_2 are both positive. Then we shrink blocks 1 and 2 by one column. If $k_3 \geqslant k_5$ and $k_3 \geqslant k_6$, we inflate blocks 5 and 6 by one column each, calling this new matrix A_2. We then have

$$\begin{aligned}
&\det(A_2 A_2^T) - \det(A_1 A_1^T) \\
&\quad = \psi(k_1 - 1, k_2 - 1, k_3, 0, k_5 + 1, k_6 + 1, k_7) \\
&\qquad - \psi(k_1, k_2, k_3, 0, k_5, k_6, k_7) \\
&\quad = k_1(k_2 - 1) + k_2(k_1 - 1) + 2k_1k_3 + 2k_2k_3 \\
&\qquad + (k_5 + k_6)(k_3 - 1) + k_5(k_3 - k_6) + k_6(k_3 - k_5) \\
&\quad \geqslant 0
\end{aligned}$$

since the terms in the last expression are all nonnegative.

If $k_6 \geqslant k_5$ and $k_6 \geqslant k_3$, then we inflate blocks 3 and 5 by one column each and call the new matrix A_2. Then

$$\begin{aligned}
&\det(A_2 A_2^T) - \det(A_1 A_1^T) \\
&\quad = \psi(k_1 - 1, k_2 - 1, k_3 + 1, 0, k_5 + 1, k_6, k_7) \\
&\qquad - \psi(k_1, k_2, k_3, 0, k_5, k_6, k_7) \\
&\quad = (k_1k_2 - 1) + k_3(k_1 - 1) + k_3(k_2 - 1) + (k_6 - k_5) \\
&\qquad + 2k_3(k_6 - k_5) + k_1k_6 + k_2k_6 + 2k_5k_6 + k_7(k_1 - 1) \\
&\qquad + k_7(k_6 - k_3) \\
&\quad \geqslant 0.
\end{aligned}$$

Again, the terms in the last expression are all nonnegative.

Similarly, if $k_5 \geqslant k_3$ and $k_5 \geqslant k_6$, we inflate blocks 3 and 6 by one column each, obtaining

$$\begin{aligned}
&\det(A_2 A_2^T) - \det(A_1 A_1^T) \\
&\quad = \psi(k_1 - 1, k_2 - 1, k_3 + 1, 0, k_5, k_6 + 1, k_7) \\
&\qquad - \psi(k_1, k_2, k_3, 0, k_5, k_6, k_7) \\
&\quad = (k_1 k_2 - 1) + k_3(k_1 - 1) + k_3(k_2 - 1) + (k_5 - k_6) \\
&\qquad + 2k_3(k_5 - k_6) + k_1 k_5 + k_2 k_5 + 2k_5 k_6 + k_7(k_1 - 1) \\
&\qquad + k_7(k_5 - k_3) \\
&\quad \geqslant 0.
\end{aligned}$$

Therefore, we may shrink blocks 1 and 2 one column at a time, inflating blocks 3, 5, and 6 as necessary until one of blocks 1 and 2 is empty.

Without loss of generality, assume $k_2 = 0$. If $k_1 > 0$ we can shrink block 1 by one column. If $k_3 \leqslant k_5$ and $k_3 \leqslant k_6$, we inflate block 3 by one column, obtaining the matrix A_3 and the following computation:

$$\begin{aligned}
&\det(A_3 A_3^T) - \det(A_2 A_2^T) \\
&\quad = \psi(k_1 - 1, 0, k_3 + 1, 0, k_5, k_6, k_7) - \psi(k_1, 0, k_3, 0, k_5, k_6, k_7) \\
&\quad = k_5(k_1 - 1) + k_6(k_1 - 1) + k_7(k_1 - 1) + k_5(k_6 - k_3) \\
&\qquad + k_6(k_5 - k_3) + k_5 k_6 + k_7(k_6 - k_3) \\
&\quad \geqslant 0.
\end{aligned}$$

If $k_5 \leqslant k_3$ and $k_5 \leqslant k_6$, we inflate block 5 by one column, obtaining

$$\begin{aligned}
&\det(A_3 A_3^T) - \det(A_2 A_2^T) \\
&\quad = \psi(k_1 - 1, 0, k_3, 0, k_5 + 1, k_6, k_7) - \psi(k_1, 0, k_3, 0, k_5, k_6, k_7) \\
&\quad = k_3(k_1 - 1) + k_6(k_1 - 1) + k_7(k_1 - 1) + k_3(k_6 - k_5) + k_6(k_3 - k_5) \\
&\qquad + k_3 k_6 + k_7(k_6 - k_5) \\
&\quad \geqslant 0.
\end{aligned}$$

If $k_6 \leqslant k_3$ and $k_6 \leqslant k_5$, we inflate block 6 by one column, obtaining

$$\begin{aligned}
&\det\left(A_3 A_3^T\right) - \det\left(A_2 A_2^T\right)\\
&\quad = \psi(k_1 - 1, 0, k_3, 0, k_5, k_6 + 1, k_7) - \psi(k_1, 0, k_3, 0, k_5, k_6, k_7)\\
&\quad = (k_3 + k_5)(k_1 - 1) + k_3(k_5 - k_6) + k_5(k_3 - k_6) + k_3 k_5\\
&\quad \geqslant 0.
\end{aligned}$$

We may then shrink block 1 by one column repeatedly until it is empty, while inflating columns 3, 5, and 6 as necessary. Therefore, if $\det(AA^T)$ is a maximum, blocks 1, 2, and 4 are all empty.

Now, suppose that blocks 1, 2, and 4 are all empty but block 7 is not. The strategy is then to shrink block 7 by one column while inflating the smallest of blocks 3, 5, or 6 by one column. Suppose, without loss of generality, that block 3 is no larger than block 5 or 6. Then we inflate block 3 by one column and compute

$$\begin{aligned}
&\det\left(A_4 A_4^T\right) - \det\left(A_3 A_3^T\right)\\
&\quad = \psi(0, 0, k_3 + 1, 0, k_5, k_6, k_7 - 1) - \psi(0, 0, k_3, 0, k_5, k_6, k_7)\\
&\quad = (k_5 + k_6)(k_7 - 1) + k_5(k_6 - k_3) + k_6(k_5 - k_3) + k_5 k_6\\
&\quad \geqslant 0.
\end{aligned}$$

It follows that block 7 may be shrunk repeatedly while inflating the smallest of blocks 3, 5, and 6 each time block 7 is shrunk. Therefore, to maximize the volume of T, blocks 1, 2, 4, and 7 must be empty. In this case, $\det(AA^T) = \psi(0, 0, k_3, 0, k_5, k_6, 0) = 4k_3k_5k_6$. Maximizing this expression with respect to the constraint $k_3 + k_5 + k_6 = d$, we find that

$$\max\left(\det\left(AA^T\right)\right) = \begin{cases} 4n^3, & \text{if } d = 3n\\ 4(n^3 + n), & \text{if } d = 3n + 1\\ 4(n^3 + 2n^2 + n), & \text{if } d = 3n + 2 \end{cases}$$

and so

$$\max(\mathrm{vol}(T)) = \begin{cases} \sqrt{n^3}/3, & \text{if } d = 3n \\ \sqrt{n^3 + n}/3, & \text{if } d = 3n + 1 \\ \sqrt{n^3 + 2n^2 + n}/3, & \text{if } d = 3n + 2 \end{cases}$$

or, if $d = 3n + i$,

$$\max(\mathrm{vol}(T)) = \sqrt{n^{3-i}(n + 1)^i}/3$$

as desired. ■

6. LARGE j-SIMPLICES IN d-CUBES FOR $4 \leqslant j \leqslant 8$

This section is devoted to the cases in which $4 \leqslant j \leqslant 8$. With a single exception, we do not determine the precise value of $\rho_{j,d}$ but we do establish lower bounds for $G(j, d)$, which can be translated into lower bounds for $\rho_{j,d}$, and we believe these lower bounds to be sharp in many cases. Here $G(j, d)$ denotes the maximum of $\det(AA^T)$ as A ranges over all $j \times d$ (0, 1) matrices. (Recall that $\rho_{j,d} = \sqrt{G(j, d)}$.)

The exception is the case (4, 10), which was discussed at the end of Section 4. Before learning of the result of [JN83] mentioned there, we conducted an exhaustive search over all 4×10 (0, 1) matrices, leading to the discovery that

$$A = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix}$$

is a matrix of this size for which $\det(AA^T)$ is maximized. For this particular A, $\det(AA^T) = 405 = G(4, 10)$. Hence $\rho_{4,10} = \sqrt{405}$, and $\sqrt{405}/24$ is the maximum volume of a 4-simplex in Q_{10}. In this case, the rows of A together with the origin form the vertex set of a regular 4-simplex of edge length $\sqrt{6}$. This shows that $4 \in R_{10}^{\exists}$. The same search showed, in fact, that every 4×10 (0, 1) matrix with Gram determinant equal to 405 determines a regular simplex whose centroid is different from that of the cube. Since these maximizing regular 4-simplices do not have their centroid at the center of the cube, this proves the following.

6.1. THEOREM. $4 \in R_{10}^{\exists} \setminus R_{10}^{c}$.

We conjecture that $4 \in R_{10}^{\forall}$. However, the computer search shows only that every *bound* largest 4-simplex in Q_{10} is regular.

In several of the search procedures described in this and later sections, the length of the search was reduced by using the result of Lubin [Lu87] (proved independently in [Hu95]) that, for any rectangular matrix A, it is possible to permute the rows and the columns of A so as to obtain a matrix in which *both* the rows and the columns are in lexicographic order.

We next establish lower bounds on the largest Gram determinants for $4 \times n$ (0, 1) matrices when $n \geqslant 10$. It is conjectured that these are the actual largest Gram determinants. In the matrices providing the lower bounds in Theorem 6.2 below, the (0, 1)-patterns were initially discovered by conducting many randomized hill-climbing searches over the set of $4 \times n$ (0, 1) matrices. Each step in the search consisted of toggling one randomly selected entry in the starting matrix A and computing the Gram determinant of the resulting matrix B. If B had a higher Gram determinant than A, the search proceeded with B in place of A; otherwise, A was left alone and other randomly chosen entries were toggled. In other words, the search was conducted in the graph of the $4 \times n$ (0, 1) matrices, with two matrices being adjacent if and only if they differ in a single entry. As would be expected from the results of Section 3, many different starts were required before the patterns emerged.

6.2. THEOREM. *For* $n = 10k + m$,

$$G(4, n) \geqslant \begin{cases} 405k^4 & \text{if } m = 0 \\ 405k^4 + 162k^3 & \text{if } m = 1 \\ 405k^4 + 324k^3 + 81k^2 + 6k & \text{if } m = 2 \\ 405k^4 + 486k^3 + 189k^2 + 24k & \text{if } m = 3 \\ 405k^4 + 648k^3 + 378k^2 + 96k + 9 & \text{if } m = 4 \\ 405k^4 + 810k^3 + 576k^2 + 174k + 19 & \text{if } m = 5 \\ 405k^4 + 972k^3 + 864k^2 + 336k + 48 & \text{if } m = 6 \\ 405k^4 + 1134k^3 + 1161k^2 + 516k + 84 & \text{if } m = 7 \\ 405k^4 + 1296k^3 + 1539k^2 + 804k + 156 & \text{if } m = 8 \\ 405k^4 + 1458k^3 + 1944k^2 + 1134k + 243 & \text{if } m = 9. \end{cases}$$

Proof. These lower bounds were obtained by concatenating k copies of the matrix A above to make the matrix A_k and adding and, in some cases, removing columns in the following prescribed manner to arrive at the matrix $\tilde{A}$: When $m = 0$, $\tilde{A} = A_k$. When $m \in \{1, 3, 4, 5, 6, 7, 9\}$, we concatenate B_m onto the end of A_k to get $\tilde{A}$ where the matrices B_m are as follows:

$$B_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \quad B_3 = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \\ 1 & 1 & 0 \end{pmatrix}, \quad B_4 = \begin{pmatrix} 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix},$$

$$B_5 = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 0 \end{pmatrix}, \quad B_6 = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 \end{pmatrix},$$

$$B_7 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \end{pmatrix},$$

$$B_9 = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 1 & 0 & 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 & 0 & 1 & 1 & 1 & 0 \end{pmatrix}.$$

When $m = 2$, we replace an occurrence of the seventh column of A with copies of the first three columns of A to get $\tilde{A}$, and when $m = 8$, we concatenate an extra copy of A and then replace the first three columns of this copy of A with a copy of the seventh column of A to get $\tilde{A}$.

If we then compute $F(4, 10k + m) = \det(\tilde{A}\,\tilde{A}^T)$ for each m we obtain the table of polynomials listed in the statement of the theorem. Therefore, $G(4, 10k + m) \geqslant F(4, 10k + m)$, which yields the stated result. ■

We showed in Section 4 that $5 \in R_{10k}$. To supplement that information, we now set forth some lower bounds on the largest Gram determinants for

$5 \times d$ $(0, 1)$ matrices for some other values of d. The patterns that are involved here were discovered by the same randomized hill-climbing technique used in connection with Theorem 6.2.

6.3. THEOREM. *For* $d = 10k + m$, $k > 2$,

$$G(5, d) \geqslant \begin{cases} 1458k^5 & \text{if } m = 0 \\ 1458k^5 + 729k^4 & \text{if } m = 1 \\ 1458k^5 + 1458k^4 + 324k^3 & \text{if } m = 2 \\ 1458k^5 + 2187k^4 + 972k^3 + 135k^2 & \text{if } m = 3 \\ 1458k^5 + 2916k^4 + 1944k^3 + 540k^2 + 54k & \text{if } m = 4 \\ 1458k^5 + 3645k^4 + 3240k^3 + 1242k^2 + 198k + 9 & \text{if } m = 5 \\ 1458k^5 + 4374k^4 + 4860k^3 + 2484k^2 + 594k + 54 & \text{if } m = 6 \\ 1458k^5 + 5103k^4 + 6804k^3 + 4266k^2 + 1242k + 135 & \text{if } m = 7 \\ 1458k^5 + 5832k^4 + 9072k^3 + 6804k^2 + 2430k + 324 & \text{if } m = 8 \\ 1458k^5 + 6561k^4 + 11664k^3 + 10206k^2 + 4374k + 729 & \text{if } m = 9 \end{cases}$$

Proof. To obtain these bounds, begin by concatenating k copies of the matrix

$$A = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}$$

to make the matrix A_k. Then concatenate B_i to A_k, where B_i is the appropriate matrix taken from those below:

$$B_1 = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 1 \end{pmatrix}, \qquad B_2 = \begin{pmatrix} 0 & 1 \\ 0 & 1 \\ 1 & 0 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}, \qquad B_3 = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{pmatrix},$$

$$B_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{pmatrix}, \qquad B_5 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 \end{pmatrix},$$

$$B_6 = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 0 & 0 \end{pmatrix}, \qquad B_7 = \begin{pmatrix} 0 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 & 0 \\ 1 & 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix},$$

$$B_8 = \begin{pmatrix} 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix},$$

$$B_9 = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 0 & 0 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 1 & 0 & 1 & 0 & 0 \end{pmatrix}. \qquad \blacksquare$$

Theorem 6.3 is concerned only with $d \geqslant 30$. For $d \leqslant 29$, we have the lower bounds on $G(5, d)$ listed below. They were obtained experimentally by using randomized hill climbing from a number of randomly chosen starting configurations. The numbers marked with an asterisk agree with those produced by the polynomials listed in the statement of Theorem 6.3, but the ones not marked are lower than the ones indicated in the theorem. This suggests that there may be anomalous low-dimensional behavior in those cases.

d	Lower Bound for $G(5, d)$
5	25
6	64
7	192
8	384
9	729*
10	1458*
11	2187*
12	3240*
13	4752*
14	6912*
15	9880
16	13975
17	19500
18	25920*
19	34992*
20	46656*
21	58320*
22	72576*
23	89964*
24	111132*
25	136269*
26	166698*
27	202752
28	244944*
29	295245*

6.4. THEOREM. *For $n = 7k + m$, $k \geqslant 2$,*

$$G(6, n) \geqslant \begin{cases} 448k^6 & \text{if } m = 0 \\ 448k^6 + 384k^5 & \text{if } m = 1 \\ 448k^6 + 768k^5 + 480k^4 + 128k^3 + 12k^2 & \text{if } m = 2 \\ 448k^6 + 1152k^5 + 1200k^4 + 640k^3 + 180k^2 + 24k + 1 & \text{if } m = 3 \\ 448k^6 + 1536k^5 + 2160k^4 + 1600k^3 + 660k^2 + 144k + 13 & \text{if } m = 4 \\ 448k^6 + 1920k^5 + 3360k^4 + 3072k^3 + 1548k^2 + 408k + 44 & \text{if } m = 5 \\ 448k^6 + 2304k^5 + 4880k^4 + 5440k^3 + 3360k^2 + 1088k + 144 & \text{if } m = 6. \end{cases}$$

Proof. First, we note that the rows of the matrix

$$A_7 = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}$$

form the remaining six vertices of a nicely regular 6-simplex in the unit 7-cube Q_7. This matrix satisfies the conditions of the theorem for $k = 1$, $m = 0$, because $\det(A_7 A_7^T) = 448$.

We note that when $m \neq 0$, the following $6 \times (14 + m)$ $(0, 1)$ matrices A_{14+m} have the Gram determinants proposed above for the case $k = 2$. To produce suitable matrices for higher k, it suffices to concatenate $k - 2$ copies of A_7 to the matrix A_{14+m}:

$$A_{15} = \begin{pmatrix} 000000111101111 \\ 010111001100101 \\ 111001000001111 \\ 011010011011001 \\ 101101101111000 \\ 110110110010110 \end{pmatrix}, \qquad A_{16} = \begin{pmatrix} 0000000011111111 \\ 0000111100001111 \\ 0111001100110011 \\ 1011110001010101 \\ 1101110010101010 \\ 1110001111001100 \end{pmatrix},$$

$$A_{17} = \begin{pmatrix} 00000001111111011 \\ 00011110000111101 \\ 01100110011001110 \\ 10101011101000101 \\ 11010101100010110 \\ 11111000010100011 \end{pmatrix}, \qquad A_{18} = \begin{pmatrix} 000000111110011111 \\ 000111000111100111 \\ 011001011001101011 \\ 101110001000111101 \\ 110010110001110110 \\ 111101100111011000 \end{pmatrix},$$

$$A_{19} = \begin{pmatrix} 0000000111111001111 \\ 0001111000011100111 \\ 0110001000110111011 \\ 1110010011001110101 \\ 1011110100110011100 \\ 1101101111000101010 \end{pmatrix}, \qquad A_{20} = \begin{pmatrix} 00000000001111111111 \\ 00001111110001100111 \\ 01110001110010111001 \\ 11110010011100000111 \\ 10011110100110011010 \\ 11101101001001011100 \end{pmatrix}.$$

■

An interesting pattern emerges when we examine the matrices $B_{14+m} = A_{14+m}A_{14+m}^T$; namely,

$$B_{14} = \begin{pmatrix} 8 & 4 & 4 & 4 & 4 & 4 \\ 4 & 8 & 4 & 4 & 4 & 4 \\ 4 & 4 & 8 & 4 & 4 & 4 \\ 4 & 4 & 4 & 8 & 4 & 4 \\ 4 & 4 & 4 & 4 & 8 & 4 \\ 4 & 4 & 4 & 4 & 4 & 8 \end{pmatrix}, \qquad B_{15} = \begin{pmatrix} 8 & 4 & 4 & 4 & 4 & 4 \\ 4 & 8 & 4 & 4 & 4 & 4 \\ 4 & 4 & 8 & 4 & 4 & 4 \\ 4 & 4 & 4 & 8 & 4 & 4 \\ 4 & 4 & 4 & 4 & 9 & 4 \\ 4 & 4 & 4 & 4 & 4 & 9 \end{pmatrix},$$

$$B_{16} = \begin{pmatrix} 8 & 4 & 4 & 4 & 4 & 4 \\ 4 & 8 & 4 & 4 & 4 & 4 \\ 4 & 4 & 9 & 4 & 4 & 4 \\ 4 & 4 & 4 & 9 & 4 & 4 \\ 4 & 4 & 4 & 4 & 9 & 4 \\ 4 & 4 & 4 & 4 & 4 & 9 \end{pmatrix}, \qquad B_{17} = \begin{pmatrix} 9 & 4 & 4 & 4 & 4 & 4 \\ 4 & 9 & 4 & 4 & 4 & 4 \\ 4 & 4 & 9 & 4 & 4 & 4 \\ 4 & 4 & 4 & 9 & 4 & 4 \\ 4 & 4 & 4 & 4 & 9 & 4 \\ 4 & 4 & 4 & 4 & 4 & 9 \end{pmatrix},$$

$$B_{18} = \begin{pmatrix} 10 & 5 & 5 & 5 & 5 & 5 \\ 5 & 10 & 5 & 5 & 5 & 5 \\ 5 & 5 & 10 & 5 & 5 & 5 \\ 5 & 5 & 5 & 10 & 5 & 5 \\ 5 & 5 & 5 & 5 & 10 & 5 \\ 5 & 5 & 5 & 5 & 5 & 11 \end{pmatrix},$$

$$B_{19} = \begin{pmatrix} 10 & 5 & 5 & 5 & 5 & 5 \\ 5 & 10 & 5 & 5 & 5 & 5 \\ 5 & 5 & 10 & 5 & 5 & 5 \\ 5 & 5 & 5 & 11 & 5 & 5 \\ 5 & 5 & 5 & 5 & 11 & 5 \\ 5 & 5 & 5 & 5 & 5 & 11 \end{pmatrix},$$

$$B_{20} = \begin{pmatrix} 10 & 5 & 5 & 5 & 5 & 5 \\ 5 & 11 & 5 & 5 & 5 & 5 \\ 5 & 5 & 11 & 5 & 5 & 5 \\ 5 & 5 & 5 & 11 & 5 & 5 \\ 5 & 5 & 5 & 5 & 11 & 5 \\ 5 & 5 & 5 & 5 & 5 & 11 \end{pmatrix}.$$

Another way to phrase this is that if I is the identity matrix, J is the matrix of all 1's, and I_l is the matrix of all 0's except for the last l diagonal elements which are all 1's, then for $k = 2$,

$$B_{14+m} = \begin{cases} 4(I+J) & \text{if } m = 0 \\ 4(I+J) + I_2 & \text{if } m = 1 \\ 4(I+J) + I_4 & \text{if } m = 2 \\ 4(I+J) + I_6 & \text{if } m = 3 \\ 5(I+J) + I_1 & \text{if } m = 4 \\ 5(I+J) + I_3 & \text{if } m = 5 \\ 5(I+J) + I_5 & \text{if } m = 6. \end{cases}$$

For higher k, the matrix A_{7k+m} arises from the concatenation of enough copies of A_7 to the proper A_{14+m}. We then obtain

$$B_{7k+m} = \left\lfloor \frac{2(7k+m)}{7} \right\rfloor (I+J) + I_{[2m \bmod 7]},$$

where $[s \bmod t]$ is used to denote the residue of s modulo t. We have therefore proved the following.

6.5. THEOREM. *For* $k \geqslant 2$,

$$G(6, 7k+m) \geqslant \det\left(\left\lfloor \frac{2(7k+m)}{7} \right\rfloor (I+J) + I_{[2m \bmod 7]} \right).$$

To evaluate the determinant in Theorem 6.5, simply apply Corollary 1.10 with the appropriate choice of parameters. The same comment applies to 6.7 and 7.4–7.7.

We conjecture that the inequality of Theorem 6.5 is in fact an equality. This formula for 6-simplices is extended in Theorem 7.7 to a formula for $(4n+2)$-simplices.

We begin our examination of largest 7-simplices in d-cubes by recalling from Section 4 that in the 7-cube there is a largest 7-simplex that is regular. One such simplex has one vertex at the origin and its other vertices are the rows of the matrix

$$C_7 = \begin{pmatrix} 0 & 0 & 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 1 & 0 & 0 & 1 & 1 \\ 0 & 1 & 1 & 1 & 1 & 0 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 & 0 & 0 & 1 \end{pmatrix}.$$

Note that $C_7 C_7^T = 2(I + J)$. If the matrix C_{7k+m} is formed by concatenating k copies of C_7 and the first m columns of C_7, then

$$\det\left(C_{7k+m} C_{7k+m}^T\right) = 1024k^{7-m}(k+1)^m.$$

This establishes the following.

6.6. THEOREM. $G(7, 7k + m) \geqslant 1024k^{7-m}(k + 1)^m$.

We conjecture that the inequality above is in fact an equality. This formula for 7-simplices is generalized in Theorem 7.1 to a formula for $(4n + 3)$-simplices.

To end Section 6, we turn our attention to the case $j = 8$. We proceed as in the case of $j = 6$, except that we can discern the $k(I + J) + I_m$ pattern only when d is even.

6.7. THEOREM. *For $m \in \{0, \ldots, 8\}$ and any integer k such that $2(9k + m) \geqslant 28$,*

$$G(8, 2(9k + m)) \geqslant \det\left((5k + \lfloor 5m/9 \rfloor)(I + J) + I_{[5m \bmod 9]}\right).$$

Proof. Consider the following (0, 1) matrices:

$$D_{18} = \begin{pmatrix} 000001111100011111 \\ 000110011111100011 \\ 011010001101111100 \\ 101100100110101101 \\ 110111000000110111 \\ 011001110011100110 \\ 101101001011011010 \\ 110010110011011001 \end{pmatrix}$$

$$D_{28} = \begin{pmatrix} 0000000000000011111111111111 \\ 0000001111111100001110001111 \\ 0001110001111100110011110001 \\ 1110010110001101010010110110 \\ 0011111110010010100100111010 \\ 1110101011100001100101010101 \\ 1111001100100110011001101001 \\ 1101110001011011001001001110 \end{pmatrix}$$

$$D_{30} = \begin{pmatrix} 000000000001111111100011111111 \\ 000001111110000001101100111111 \\ 001110000110000110111111000111 \\ 010110111000011000010111011011 \\ 111011000010101000000111111100 \\ 110100111011100110111001101000 \\ 111001011101011011011010000101 \\ 101111100101110101010100110010 \end{pmatrix}$$

$$D_{32} = \begin{pmatrix} 00000000000011111111111100011111 \\ 00000111111100000001111101100111 \\ 11111000001100011110000101100111 \\ 00111000110100100110111011111000 \\ 11001011011001100011000110111001 \\ 01010111100110011101000011011001 \\ 11100100111011101000001011001110 \\ 10111111000011010000110010110110 \end{pmatrix}$$

$$D_{34} = \begin{pmatrix} 0000000000000111111111000111111111 \\ 0000001111111000000011011001111111 \\ 0001110000111000011100111110001111 \\ 0110110011000011100000111010110111 \\ 1001011101011101100101101110110000 \\ 1111111100100110100010001101001011 \\ 1111000111100101011001110011001100 \\ 1110101010011010011110110101110000 \end{pmatrix}$$

$$D_{36} = \begin{pmatrix} 000001111100011111000000111110001111 \\ 000110011111100011000110011111100011 \\ 011010001101111100011010001101111100 \\ 101100100110101101101100100110101101 \\ 110111000000110111110111000000110111 \\ 011001110011100110011001110011100110 \\ 101101001011011010101101001011011010 \\ 110010110011011001110010110011011001 \end{pmatrix}$$

$$D_{38} = \begin{pmatrix} 00000000000000001111111111000111111111 \\ 00000001111111100000000011011001111111 \\ 00011110000011100000111001111100011111 \\ 11100110001101101111000011010100100111 \\ 01111010111110010011000101001101011001 \\ 10101101011110000101111000111111100000 \\ 11011111110000011100001101100010101110 \\ 11110001100001111010110011111011010000 \end{pmatrix}$$

$$D_{40} = \begin{pmatrix} 0000000000001111111111100000011111111111 \\ 0000000111110000011111111111100000011111 \\ 0001111000110011100001101111100111100011 \\ 0110011001010101100110010111111001101100 \\ 1001111111001000101000001001111010111101 \\ 1111100000101100010010111011111100110010 \\ 1110001111000011011000011110011111000011 \\ 1111110110111110000101010100000111011100 \end{pmatrix}$$

$$D_{42} = \begin{pmatrix} 000000000000000000111111111110001111111111 \\ 000000000111111110000000001111110001111111 \\ 000111111000011110000111100101101100001111 \\ 011001111111100000111000100101110100110011 \\ 111110111001100011001011000010000011111101 \\ 101010001110011110111101000010111111010000 \\ 110101010011100101010110011011111101000100 \\ 111111100100011001100000111011011010101010 \end{pmatrix}$$

$$D_{44} = \begin{pmatrix} 00000000000000111111111111100000011111111111 \\ 00000001111111000000001111011111000001111111 \\ 00011110000011001111100001111111000110001111 \\ 01100110011100010001100110101111011110110001 \\ 11111010100101100000011000010011111110010111 \\ 11101001101010010110000010110101101111101010 \\ 11111010110101110001010011010101100010111100 \\ 10010111110101101111010100111100111001100000 \end{pmatrix}$$

Then, letting $E_n = D_n D_n^T$, we have

$$E_{28} = 7(I + J) + I_7$$

$$E_{30} = 8(I + J) + I_3$$

$$E_{32} = 8(I + J) + I_8$$

$$E_{34} = 9(I + J) + I_4$$

$$E_{36} = 10(I + J) + I_0$$

$$E_{38} = 10(I + J) + I_5$$

$$E_{40} = 11(I + J) + I_1$$

$$E_{42} = 11(I + J) + I_6$$

$$E_{44} = 12(I + J) + I_2,$$

which confirms the theorem in these cases. For higher values of k, the proof is completed by concatenating an appropriate number of copies of D_{18} to the correct D_{18k+2m} above. ■

A higher-dimensional analogue of this result appears in Theorem 7.6.

7. LARGE HIGHER-DIMENSIONAL NONREGULAR j-SIMPLICES RELATED TO HADAMARD MATRICES

Section 4 was concerned with the relationship between H-matrices and regular largest simplices in d-cubes. Here, we concentrate on finding large (possibly largest) simplices that are not regular but nevertheless have a close relationship to H-matrices.

A (0, 1) matrix A is here called *k-regular* when $AA^T = k(I + J)$, or simply *regular* when the value of k is apparent. Note that if A is a k-regular $j \times d$ matrix, then the rows of A, when taken along with the origin 0, form the vertex set of a bound regular j-simplex of edge length $\sqrt{2k}$ in Q_d.

We look first at the case where $j = 4k - 1$. The following is an analogue of Theorem 6.6.

7.1. THEOREM. *If $4k$ is an H-number, then for $p \geqslant 1$, $q \in \{0, 1, \ldots, +4k - 2\}$,*

$$G(4k - 1, (4k - 1)p + q) \geqslant 4k^{4k} p^{4k-1-q}(p + 1)^q.$$

Proof. Since $4k$ is an H-number, there is a regular $(4k - 1) \times (4k - 1)$ (0, 1)-matrix A from Theorem 2.4. Furthermore, A^T is regular as well, since both A and A^T correspond to H-matrices in the construction of Theorem 2.4. It follows that $AA^T = A^TA = k(I + J)$.

Now, form a $(4k - 1) \times ((4k - 1)p + q)$ matrix $A_{(4k-1)p+q}$ by concatenating p full copies of A and a single copy of the matrix A_q formed by the first q columns of A. Then set

$$B = A_{(4k-1)p+q} A^T_{(4k-1)p+q} = p(AA^T) + A_q A_q^T.$$

Our objective is now to find the determinant of B, and for that purpose we compute the product of B's eigenvalues.

Denote the ith column of A by a_i, and note that since $A^TA = k(I + J)$, $a_i \cdot a_i = 2k$ and $a_i \cdot a_j = k$ if $i \neq j$. We then calculate $B(a_1 - a_i)$ for $1 < i \leqslant q$:

$$\begin{aligned} B(a_1 - a_i) &= \left(pAA^T + A_q A_q^T\right)(a_1 - a_i) \\ &= pA\begin{pmatrix} a_1 \cdot a_1 - a_1 \cdot a_i \\ \vdots \\ a_{4k-1} \cdot a_1 - a_{4k-1} \cdot a_i \end{pmatrix} + A_q \begin{pmatrix} a_1 \cdot a_1 - a_1 \cdot a_i \\ \vdots \\ a_q \cdot a_1 - a_q \cdot a_i \end{pmatrix} \\ &= p(ka_1 - ka_i) + (ka_1 - ka_i) \\ &= (p + 1)k(a_1 - a_i). \end{aligned}$$

Hence the vectors $a_1 - a_i$ $(1 < i \leqslant q)$ are eigenvectors of B, each with eigenvalue $(p + 1)k$.

For $q + 1 \leqslant i < 4k - 1$, we have

$$\begin{aligned} B(a_{4k-1} - a_i) &= \left(pAA^T + A_q A_q^T\right)(a_{4k-1} - a_i) \\ &= pA\begin{pmatrix} a_1 \cdot a_{4k-1} - a_1 \cdot a_i \\ \vdots \\ a_{4k-1} \cdot a_{4k-1} - a_{4k-1} \cdot a_i \end{pmatrix} + A_q \begin{pmatrix} a_1 \cdot a_{4k-1} - a_1 \cdot a_i \\ \vdots \\ a_q \cdot a_{4k-1} - a_q \cdot a_i \end{pmatrix} \\ &= p(ka_{4k-1} - ka_i) + 0 \\ &= pk(a_{4k-1} - a_i). \end{aligned}$$

Hence the vectors $a_{4k-1} - a_i$ $(q + 1 \leqslant i < 4k - 1)$ are eigenvectors of B, each with eigenvalue pk.

To find the product of the other two eigenvalues, λ_1 and λ_2, say, we note that the vectors $\mathbf{v} = a_1 + \cdots + a_q$ and $\mathbf{w} = a_{q+1} + \cdots + a_{4k-1}$ are orthogonal to the eigenvectors found above. We have

$$\begin{aligned} B\mathbf{v} &= \left(pAA^T + A_q A_q^T\right)\mathbf{v} \\ &= pA\begin{pmatrix} a_1 \cdot a_1 + \cdots + a_1 \cdot a_q \\ \vdots \\ a_{4k-1} \cdot a_1 + \cdots + a_{4k-1} \cdot a_q \end{pmatrix} + A_q \begin{pmatrix} a_1 \cdot a_1 + \cdots + a_1 \cdot a_q \\ \vdots \\ a_q \cdot a_1 + \cdots + a_q \cdot a_q \end{pmatrix} \\ &= p(q+1)k\mathbf{v} + pqk\mathbf{w} + k(q+1)\mathbf{v}, \end{aligned}$$

and

$$\begin{aligned} B\mathbf{w} &= \left(pAA^T + A_q A_q^T\right)\mathbf{w} \\ &= pA\begin{pmatrix} a_1 \cdot a_{q+1} + \cdots + a_1 \cdot a_{4k-1} \\ \vdots \\ a_{4k-1} \cdot a_{q+1} + \cdots + a_{4k-1} \cdot a_{4k-1} \end{pmatrix} \\ &\quad + A_q \begin{pmatrix} a_1 \cdot a_{q+1} + \cdots + a_1 \cdot a_{4k-1} \\ \vdots \\ a_q \cdot a_{q+1} + \cdots + a_q \cdot a_{4k-1} \end{pmatrix} \\ &= p(4k-1-q)k\mathbf{v} + p(4k-q)k\mathbf{w} + k(4k-1-q)\mathbf{v}. \end{aligned}$$

If $b\mathbf{v} + \mathbf{w}$ is an eigenvector with eigenvalue λ, then

$$\begin{aligned} B(b\mathbf{v} + \mathbf{w}) &= b(p(q+1)k\mathbf{v} + pqk\mathbf{w} + k(q+1)\mathbf{v}) \\ &\quad + p(4k-1-q)k\mathbf{v} + p(4k-q)k\mathbf{w} + k(4k-1-q)\mathbf{v} \\ &= (b(q+1) + (4k-1-q))(p+1)k\mathbf{v} \\ &\quad + (bq + 4k - q)pk\mathbf{w} \\ &= \lambda b\mathbf{v} + \lambda\mathbf{w}. \end{aligned}$$

Therefore, $\lambda b = (b(q+1) + (4k-1-q))(p+1)k$ and $\lambda = (bq + 4k - q)pk$. Eliminating b from these equations, we obtain

$$\lambda^2 - (pk(4k-q) + (q+1)(p+1)k)\lambda + (4k)k^2p(p+1) = 0.$$

It follows that $\lambda_1\lambda_2 = (4k)k^2p(p+1)$ and hence the product of all of B's eigenvalues is

$$(kp)^{4k-1-q-1}(k(p+1))^{q-1}(4k)k^2p(p+1) = 4k^{4k}p^{4k-1-q}(p+1)^q,$$

which is the determinant of B. Therefore,

$$G(4k-1, p(4k-1)+q) \geqslant \det(B) = 4k^{4k}p^{4k-1-q}(p+1)^q$$

as desired. ■

Our repeated hill-climbing searches have led to the observation that for even j and sufficiently large d, the Gram matrix of a "largest" j-simplex in a $(d+2)$-cube differs from that of some "largest" j-simplex in a d-cube by a piece of the identity matrix. We include the quotes since we have no proof that these simplices are indeed largest. We have already seen this phenomenon in the case where $j \in \{6, 8\}$ in Theorems 6.5 and 6.7. We now set out to show a relationship between $G(2k, 2d)$ and $\det(p(I+J) + I_r)$ for certain values of p and q that depend on k and d.

We consider the $j \times (k-1)$ matrix A and the $j \times (k+1)$ matrix B below, where each matrix has $k+1$ nonzero rows:

$$A = \begin{pmatrix} 1 & \cdots & 1 \\ 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \\ 1 & \cdots & 1 \\ 0 & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 1 & \cdots & 1 & 1 \\ 1 & 0 & \cdots & 1 & 1 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 1 & 1 & \cdots & 0 & 1 \\ 1 & 1 & \cdots & 1 & 0 \\ 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 & 0 \end{pmatrix}.$$

We then note that $BB^T - AA^T = I_{k+1}$. This observation leads to the following lemma, which is proved by replacing the occurrence of A in M with B to obtain M'.

7.2. LEMMA. *If M is a $j \times p$ matrix with A as a submatrix, then there is a $j \times (p + 2)$ matrix M' such that $M'(M')^T = MM^T + I_{k+1}$.*

Next, we show the following.

7.3. LEMMA. *If M is a $j \times d$ $(0, 1)$ matrix such that $MM^T = h(I + J) + I_l$ with $l > 0$, then there exists a $j \times d$ $(0, 1)$ matrix $\tilde{M}$ such that $\tilde{M} = (h + 1)(I + J) - I_{j+1-l}$. Furthermore, the matrices M and $\tilde{M}$ have the same Gram determinant.*

Proof. Let S denote the j-simplex whose vertices are the rows of the matrix M. The idea behind this proof is to move a suitable vertex of S to the origin by a series of reflections. The resulting simplex will then have nonzero vertices that form the rows of $\tilde{M}$.

Consider row m of M. For each n, if $M_{mn} = 1$, change every entry in the nth column from 0 to 1 or vice versa. This has the effect of reflecting the simplex S in the hyperplane $x_n = \frac{1}{2}$, and that does not affect the volume of S. Let v_i' denote the location of v_i after all of the required reflections are done.

Let N be the matrix whose rows are the changed rows of M with the exception of the mth row of N, which we let be the mth row of M. Once all of these reflections are accomplished, vertex v_m will have moved to the origin and the origin will have moved to v_m. Therefore, N will be the matrix whose rows are the nonzero vertices of the final image of S.

Next, we need to determine the entries in NN^T. Recall that $(NN^T)_{pq} = v_p' \cdot v_q'$. Since $v_m' = v_m$, $(NN^T)_{mm} = (MM^T)_{mm}$.

If $p \neq m$, then we claim $(NN^T)_{pm} = (NN^T)_{mp} = v_m \cdot (v_m - v_p) = (MM^T)_{mm} - (MM^T)_{mp}$. The first equality follows from the fact that NN^T is symmetric and the last follows from the definition of MM^T. For the second equality, we note that

$$\begin{aligned}
(NN^T)_{mp} &= v_m' \cdot v_p' \\
&= v_m \cdot v_p' \\
&= \sum_i v_{mi} v_{pi}' \\
&= \sum_{\{i:\, v_{mi}=1\}} v_{mi} v_{pi}' + \sum_{\{i:\, v_{mi}=0\}} v_{mi} v_{pi}'
\end{aligned}$$

$$= \sum_{\{i:\, v_{mi}=1\}} v_{mi}(v_{mi} - v_{pi}) + \sum_{\{i:\, v_{mi}=0\}} v_{mi}v_{pi}$$

$$= \sum_{\{i:\, v_{mi}=1\}} v_{mi}(v_{mi} - v_{pi}) + \sum_{\{i:\, v_{mi}=0\}} v_{mi}(v_{mi} - v_{pi})$$

$$= \sum_{i} v_{mi}(v_{mi} - v_{pi})$$

$$= v_m \cdot (v_m - v_p),$$

proving the claim.

We next claim that for $p, q \neq m$, $v'_p \cdot v'_q = (v_p - v_m) \cdot (v_q - v_m)$. Indeed,

$$v'_p \cdot v'_q = \sum_i v'_{pi} v'_{qi}$$

$$= \sum_{\{i:\, v_{mi}=1\}} (v_{mi} - v_{pi})(v_{mi} - v_{qi}) + \sum_{\{i:\, v_{mi}=0\}} v_{pi}v_{qi}$$

$$= \sum_{\{i:\, v_{mi}=1\}} (v_{mi} - v_{pi})(v_{mi} - v_{qi}) + \sum_{\{i:\, v_{mi}=0\}} (v_{mi} - v_{pi})(v_{mi} - v_{qi})$$

$$= \sum_i (v_{mi} - v_{pi})(v_{mi} - v_{qi})$$

$$= (v_m - v_p) \cdot (v_m - v_q),$$

as desired.

Therefore, we have, for $p, q \neq m$, that

$$(NN^T)_{pq} = (v_m - v_p) \cdot (v_m - v_q)$$

$$= (MM^T)_{mm} - (MM^T)_{pm} - (MM^T)_{mq} + (MM^T)_{pq}.$$

Now, since we assumed $MM^T = h(I + J) + I_l$, we let $m = 1$, compute N, and use the claims above to find that

$$(NN^T)_{11} = (MM^T)_{11} = 2h + 1;$$

for $p = 2, \ldots, l$,

$$\begin{aligned}(NN^T)_{pp} &= (MM^T)_{11} - (MM^T)_{p1} - (MM^T)_{1p} + (MM^T)_{pp}\\ &= (2h+1) - h - h + (2h+1)\\ &= 2h+2;\end{aligned}$$

for $p = l+1, \ldots, j$,

$$\begin{aligned}(NN^T)_{pp} &= (MM^T)_{11} - (MM^T)_{p1} - (MM^T)_{1p} + (MM^T)_{pp}\\ &= (2h+1) - h - h + 2h\\ &= 2h+1;\end{aligned}$$

for $p \neq 1$,

$$\begin{aligned}(NN^T)_{p1} = (NN^T)_{1p} &= (MM^T)_{11} - (MM^T)_{1p}\\ &= (2h+1) - h\\ &= h+1;\end{aligned}$$

and for any $p \neq 1$ and $q \neq 1$ such that $p \neq q$,

$$\begin{aligned}(NN^T)_{pq} &= (MM^T)_{11} - (MM^T)_{p1} - (MM^T)_{1q} + (MM^T)_{pq}\\ &= (2h+1) - h - h + h\\ &= h+1.\end{aligned}$$

Piecing all of these together, we find that

$$NN^T = \begin{pmatrix} 2h+1 & h+1 & \cdots & h+1 & h+1 & \cdots & h+1\\ h+1 & 2h+2 & \cdots & h+1 & h+1 & \cdots & h+1\\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots\\ h+1 & h+1 & \cdots & 2h+2 & h+1 & \cdots & h+1\\ h+1 & h+1 & \cdots & h+1 & 2h+1 & \cdots & h+1\\ \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots\\ h+1 & h+1 & \cdots & h+1 & h+1 & \cdots & 2h+1 \end{pmatrix}.$$

Note that $j + 1 - l$ of the diagonal entries are equal to $2h + 1$.

If we permute the rows of N so that each of the first $j + 1 - l$ rows has $2h + 1$ 1's, and then call the resulting matrix $\tilde{M}$, we find that $(\tilde{M}\tilde{M}^T) = (h + 1)(I + J) - I_{j+1-l}$ as desired. Since row permutation does not affect Gram determinants, $\det(\tilde{M}\tilde{M}^T) = \det(NN^T) = \det(MM^T)$, completing the proof of Lemma 7.3. ■

7.4. LEMMA. *Suppose that $8k + 4$ is an H-number and p is an integer with $0 \leqslant p \leqslant 4k$. Let $m_0 = 2k - 1$, and $m_p = p(2k - 1)$ if $1 \leqslant p \leqslant 4k$. Then there exists a $(4k) \times (2p + (8k + 2)m_p)$ matrix C_{2p} for which*

$$C_{2p}C_{2p}^T = \left((2k + 1)m_p + \left\lfloor \frac{(2k + 1)p}{4k + 1} \right\rfloor\right)(I + J) + I_{[(2k+1)p \bmod 4k+1]}.$$

Proof. By Theorem 4.10, $4k + 1 \in R_{8k+2}^c$, and hence there exists a regular $(4k + 1) \times (8k + 2)$ (0, 1) matrix M associated with a largest $(4k - 1)$-simplex in Q_{8k+2}. From the construction in 4.10, each column of M has $2k + 1$ 1's and $MM^T = (2k + 1)(I + J)$. Remove the first row from M, and call the remaining matrix N. Then $NN^T = (2k + 1)(I + J)$ with one fewer row and column. Furthermore, since the first row of M is guaranteed to have at least one 0, there is at least one column of N with $2k + 1$ 1's. Permute the rows of N so that this column is $(1_{2k+1}, 0_{2k-1})^T$.

Concatenate $2k - 1$ copies of N to form a $4k \times (8k + 2)(2k - 1)$ matrix C_0. We note that $C_0C_0^T = (2k - 1)(2k + 1)(I + J)$, and so if $2p = 0$ in the statement of the lemma, then $m_0 = 2k - 1$. Thus the lemma holds for $2p = 0$.

Next, to generate the matrix C_2, we remove $2k - 1$ occurrences of the column $(1_{2k+1}, 0_{2k-1})^T$ in C_0 and concatenate the appropriate block B as in Lemma 7.2. We then obtain a $4k \times ((2k - 1)(8k + 2) + 2)$ matrix, which we call C_2. We note that $C_2C_2^T = ((2k - 1)(2k + 1))(I + J) + I_{2k+1}$, also from Lemma 7.2, and so $m_1 = 2k - 1$.

We then proceed inductively as follows: Suppose, for p, we have the matrix C_{2p} and m_p such that

$$C_{2p}C_{2p}^T = \left((2k + 1)m_p + \left\lfloor \frac{(2k + 1)p}{4k + 1} \right\rfloor\right)(I + J) + I_{[(2k+1)p \bmod 4k+1]}.$$

If $l = [(2k + 1)p \bmod 4k + 1] \leqslant 2k - 1$, then permute the rows of C_{2p} so that the first $2k + 1$ rows of C_{2p} have $2h$ ones and the next l rows of C_{2p} have $2h + 1$ ones where $h = (2k + 1)m_p + \lfloor(2k + 1)p/(4k + 1)\rfloor$. Then concatenate a copy of C_2 onto the permuted version of C_{2p} to obtain $C_{2(p+1)}$. Then

$$C_{2(p+1)}C_{2(p+1)}^T = (h + (2k-1)(2k+1))(I+J) + I_{(l+2k+1)}.$$

We then compute

$$\begin{aligned} l + 2k + 1 &= \left[(2k+1)p \bmod (4k+1)\right] + 2k + 1 \\ &= \left[(2k+1)(p+1) \bmod (4k+1)\right]. \end{aligned}$$

Also,

$$\begin{aligned} &h + (2k-1)(2k+1) \\ &\quad = (2k+1)m_p + \left\lfloor \frac{(2k+1)p}{4k+1} \right\rfloor + (2k-1)(2k+1) \\ &\quad = (2k+1)(m_p + 2k - 1) + \left\lfloor \frac{(2k+1)(p+1)}{4k+1} \right\rfloor \end{aligned}$$

since $[(2k+1)p \mod 4k+1] \leqslant 2k-1$ implies $\lfloor (2k+1)p/(4k+1) \rfloor = \lfloor (2k+1)(p+1)/(4k+1) \rfloor$. It follows that

$$\begin{aligned} C_{2(p+1)}C_{2(p+1)}^T = &\left((2k+1)(m_p + 2k - 1) + \left\lfloor \frac{(2k+1)(p+1)}{4k+1} \right\rfloor\right) \\ &\times (I+J) + I_{[(2k+1)(p+1) \bmod (4k+1)]}. \end{aligned}$$

Therefore, the induction is completed in this case with $m_{p+1} = m_p + 2k - 1$.

If $l = [(2k+1)p \mod (4k+1)] \geqslant 2k$, then concatenate a copy of C_2 onto the matrix $\tilde{C}_{2p}$ produced by Lemma 7.3, and call the resulting matrix D. We have

$$\tilde{C}_{2p}\tilde{C}_{2p}^T = (h+1)(I+J) - I_{(4k+1-l)},$$

where $h = (2k+1)m_p + \lfloor (2k+1)p/(4k+1) \rfloor$ as before. Since $4k+1-l \leqslant 2k+1$, we can suitably permute the rows of D to obtain a matrix

$C_{2(p+1)}$ such that

$$C_{2(p+1)}C_{2(p+1)}^T = (h + 1 + (2k-1)(2k+1))(I+J) + I_{(l-2k)}.$$

This time,

$$\begin{aligned} l - 2k &= [(2k+1)p \bmod 4k+1] - 2k \\ &= [(2k+1)p - 2k \bmod 4k+1] \\ &= [(2k+1)p + 2k + 1 \bmod 4k+1] \\ &= [(2k+1)(p+1) \bmod 4k+1] \end{aligned}$$

and

$$\begin{aligned} &h + 1 + (2k-1)(2k+1) \\ &\quad = (2k+1)m_p + 1 + \left\lfloor \frac{(2k+1)p}{4k+1} \right\rfloor + (2k-1)(2k+1) \\ &\quad = (2k+1)(m_p + 2k - 1) + \left\lfloor \frac{(2k+1)(p+1)}{4k+1} \right\rfloor \end{aligned}$$

since $[(2k+1)p \bmod 4k+1] \geqslant 2k$ implies $\lfloor (2k+1)p/(4k+1) \rfloor + 1 = \lfloor (2k+1)(p+1)/(4k+1) \rfloor$. Hence the induction is completed in this case as well, with $m_{p+1} = m_p + 2k - 1$.

Thus, Lemma 7.4 is proved with $m_0 = 2k - 1$ and $m_p = p(2k-1)$ for $p > 0$. ■

7.5. THEOREM. *Suppose that $8k+4$ is an H-number, and p and r are integers such that $0 \leqslant p \leqslant 4k$ and $r \geqslant m_{4k} = 8k(2k-1)$. Then there exists a $4k \times ((8k+2)r + 2p)$ $(0,1)$ matrix A such that*

$$AA^T = \left(r(2k+1) + \left\lfloor \frac{(2k+1)p}{4k+1} \right\rfloor \right)(I+J) + I_{[(2k+1)p \bmod (4k+1)]}.$$

Of course, $G(4k, (8k+2)r + 2p) \geqslant \det(AA^T)$.

Proof. Produce a matrix D by concatenating the matrix C_{2p} of Lemma 7.4 and q copies of the matrix N taken from the proof of Lemma 7.3. Then

$$DD^T = \left((q + m_p)(2k + 1) + \left\lfloor \frac{(2k + 1)p}{4k + 1} \right\rfloor\right)(I + J)$$

$$+ I_{[(2k+1)p \bmod (4k+1)]}.$$

To obtain the desired matrix A, choose q such that $q + m_p = r$. ■

We may use a similar procedure when the simplex is of dimension $4k - 2$. The following is analogous to Lemma 7.4.

7.6. Lemma. *If $4k$ is an H-number, then for each even integer $2p$ between 0 and $8k - 4$, there is some m_p such that a $(4k - 2) \times (2p + (4k - 1)m_p)$ matrix C_{2p} exists, which satisfies*

$$C_{2p}C_{2p}^T = \left(km_p + \left\lfloor \frac{2kp}{4k - 1} \right\rfloor\right)(I + J) + I_{[2kp \bmod 4k - 1]}.$$

Proof. This time we start from a regular $(4k - 1) \times (4k - 1)$ matrix. Removing its last row and suitably permuting the remaining rows yields a regular $(4k - 2) \times (4k - 1)$ matrix, which will serve the same purpose as the N as in the proof of Lemma 7.3. This N satisfies $NN^T = k(I + J)$. We then concatenate $2k - 2$ copies of N together to get C_0, and we construct C_2 by performing the replacement operation indicated in Lemma 7.1. From these operations, we obtain $m_0 = m_1 = 2k - 2$. We may then construct C_{2p+2} from C_{2p} in precisely the same fashion as in the proof of Lemma 7.4. These constructions inductively yield

$$C_{2p}C_{2p}^T = \left(km_p + \left\lfloor \frac{2kp}{4k - 1} \right\rfloor\right)(I + J) + I_{[2kp \bmod 4k - 1]}$$

with $m_p = p(2k - 2)$ as desired. ■

We can now prove the following result, which should be compared with Theorem 6.5.

7.7. THEOREM. *Suppose that $4k$ is an H-number, and q and r are integers such that $0 \leqslant q \leqslant 4k-2$ and $r \geqslant m_{4k-2}+1 = 8k(2k-2)+1$. Then there exists a $(4k-2) \times ((4k-1)r+q)$ $(0,1)$ matrix A such that*

$$AA^T = \left(rk + \left\lfloor \frac{kq}{4k-1} \right\rfloor\right)(I+J) + I_{[kq \bmod (4k-1)]}.$$

Of course, $G(4k-2,(4k-1)r+q) \geqslant \det(AA^T)$.

Proof. Fix $q \in \{0,\dots,4k-2\}$. There is some $p \in \{0,\dots,4k-2\}$ such that $q \equiv 2p \bmod (4k-1)$. From Lemma 7.6, we then have some $(4k-2) \times m_p$ matrix C_{2p} such that

$$C_{2p}C_{2p}^T = \left(km_p + \left\lfloor \frac{2kp}{4k-1} \right\rfloor\right)(I+J) + I_{[2kp \bmod 4k-1]}.$$

If $q = 2p$ then

$$C_{2p}C_{2p}^T = \left(km_p + \left\lfloor \frac{kq}{4k-1} \right\rfloor\right)(I+J) + I_{[kq \bmod 4k-1]},$$

while if $q = 2p - 4k + 1$ then

$$C_{2p}C_{2p}^T = \left(k(m_p+1) + \left\lfloor \frac{kq}{4k-1} \right\rfloor\right)(I+J) + I_{[kq \bmod (4k-1)]}.$$

Since $m_p \leqslant m_{4k-2}$, we may obtain the desired matrix A by concatenating to C_{2p} the appropriate number of copies (either $r - m_p$ or $r - m_p - 1$) of the regular $(4k-2) \times (4k-1)$ matrix N in the proof of Lemma 7.6. ■

8. ADDITIONAL COMMENTS AND PROBLEMS

The comments in this section are all related to the material of previous sections, but they have little direct relation to each other. Hence the section is divided into subsections, each with its own heading.

A. *Number of Bound j-Simplices in a d-Cube*

For each j and d with $1 \leqslant j \leqslant d$, there are $\binom{2^d}{j+1}$ $(j+1)$-sets of vertices of a d-cube, but when $j \geqslant 3$ some of these $(j+1)$-sets lie in a flat of dimension less than j and hence fail to determine a j-simplex. For a given d

and j, how many of the mentioned $(j+1)$-sets do in fact determine a j-simplex? For the case $j = d$, this problem was posed in [Ra79] by Raktoe, who supplied some earlier references and reported some results for small values of d. For the essentially equivalent matrix-theoretic problem—finding the probability that a random $n \times n(\pm 1)$ matrix is singular—the best asymptotic results are those of Kahn et al. [KKS95].

B. Simplices of Intermediate Volume

A remark of Brenner and Cummings [BC72] amounts to the conjecture that if β_d is the volume of a largest d-simplex in the unit d-cube Q_d, then for each integer k with $1 \leqslant k \leqslant d!\beta_d$ the cube has a bound d-simplex whose volume is $k/d!$. Apparently there has been no systematic attack on this problem. However, the attainment of certain values for the volume can be deduced from various arguments used to establish a lower bound on β_d. In particular, Foster [Fo66] shows that the dth Fibonacci number is always attained as a value of k.

C. Simplices, Jung's Theorem, and H-Matrices

A theorem of Jung [Ju01] asserts that if S is any set of unit diameter in Euclidean d-space $\mathbb{R}^d$, then S is contained in a ball of radius $\sqrt{d/(2d+2)}$; further, a smaller radius suffices unless the closed convex hull of S contains a regular d-simplex of unit edge length. That led to defining the *Jung constant* J_X of an arbitrary normed linear space X as the minimum ρ such that every subset S of X of diameter 1 is contained in a ball of radius ρ. An easy consequence of Helly's theorem is that when X is d-dimensional, the minimum is not reduced when S is permitted to range only over d-simplices of diameter 1. (See [DGK63] for the history of Jung's theorem, Helly's theorem, and many of their relatives.) It was proved by Bohnenblust [Bo38] and Leichtweiss [Le55] that for each d-dimensional X, $J_X \leqslant d/(d+1)$, and Leichtweiss showed further that if B is the unit ball of X, then $J_X = d/(d+1)$ with equality if and only if X contains a d-simplex S such that $S - S \subset B \subset (d+1)S$. Dolnikov [Do87] showed that when X is the d-dimensional l_1-space, this last condition is satisfied if and only if $d+1$ is an H-number. Pichugov [Pi88] established an upper bound for the Jung constant in a d-dimensional l_p-space $(1 \leqslant p \leqslant \infty)$ and showed that equality holds whenever $d+1$ is an H-number. For further information about the relationship between Jung constants and H-matrices, see [Fr91].

D. Largest 0-Orthoregular Simplices

When S is a j-simplex in $\mathbb{R}^d$, let us say that S is *v-orthoregular* provided that v is a vertex of S, the $(j-1)$-face of S that misses v is a regular

$(j-1)$-simplex, and the j edges of S that are incident to v are mutually perpendicular. It turns out that the largest 0-orthoregular d-simplices in the cube $[-1,1]^d$ are relevant to a problem concerning the growth of pivots in Gaussian elimination with complete pivoting. (See [PC83, DP88] for the original observations, and see Section 9.8 of [GK95] for the geometric formulation and for additional references.)

E. Largest Simplices and Conference Matrices

The literature contains a number of papers on maximizing the determinant of a square $(0,1)$, (± 1), or $(0, \pm 1)$ matrix subject to additional restrictions on the number and placement of certain entries (e.g., [Ry56, BS86]). Of these efforts, the one of greatest interest from our geometric viewpoint is that of maximizing the determinant of an $n \times n$ matrix whose entries are all ± 1 except that all the entries on the main diagonal are all 0. If $f(n)$ denotes the maximum attainable by the determinant of such an $n \times n$ matrix, then $f(n)$ is just $n!$ times the maximum volume of an n-simplex in $[-1,1]$ that has one vertex at the origin and whose other n vertices form a system of distinct representatives for the n coordinate hyperplanes. It is easy to see that $f(n) \leqslant (n-1)^{n/2}$, and when this upper bound is attained the matrix in question is called a *conference matrix*. The study of such matrices was initiated by Belevitch [Be50,68]. When the bound is attained, n must be even. See the papers of Delsarte, Goethals, and Seidel [GS67, DGS71] for results and conjectures concerning this situation. For odd n the problem of determining $f(n)$ is still more difficult. It has been proved recently by Bussemaker et al. [BKMS95] that $f(3) = 2$, $f(5) = 22$, $f(7) = 394$, $f(9) = 8760$, and $f(11) = 240{,}786$.

F. A Ratio Involving Largest Simplices

For a centrally symmetric d-body C with 0 as center, let $f(C)$ denote the ratio σ_0/σ, where σ_0 (resp. σ) is the volume of a 0-largest (resp. largest) d-simplex in C. Reference [GKL95] raises the problem of determining the range of $f(C)$ as C ranges over centrally symmetric d-bodies, and the problem of determining the d-bodies C for which the extreme values of $f(C)$ are attained. Also, the determination of $f(C)$ appears to be difficult for most specific choices of C, including the case $C = Q_d$.

G. Smallest d-Simplex Containing a d-Cube

In Section 2 we discussed the difficult problem of finding a largest d-simplex contained in the d-cube Q_d. The problem of finding a smallest d-simplex containing Q_d is also of interest. A theorem of [Kl86] asserts that for each smallest (or even "locally smallest") d-simplex S containing a given convex body C, the centroid of each facet of S belongs to C. However, this information must be augmented by additional geometric conditions on S in order to obtain a reasonable algorithm for actually finding a smallest containing simplex. (See [GKL95] for references to low-dimensional algorithms that deal with the problem of finding a smallest d-simplex containing a given convex d-polytope.)

H. Largest Regular j-Polytopes in Regular d-Polytopes

Of course one may ask, for every pair (C, K) consisting of a j-dimensional convex body B and a d-dimensional convex body K in $\mathbb{R}^d$, what is the largest body that is similar to C and can be placed in K? Problems of this sort are surveyed in [GK95]. This problem is especially interesting when B and K are regular polytopes. For the case in which $j = d = 3$, the six unsettled cases are those in which the pair (C, K) is (Q, I), (D, O), (T, I), (D, T), (D, I), (I, D). (Here T, Q, O, D and I denote the regular tetrahedron, cube, octahedron, dodecahedron, and cube respectively.) The remaining 14 cases were settled by Croft [Cr80] (see also [CFG91]).

Our Sections 4–6 produce certain pairs (j, d) for which the largest j-simplices contained in a given d-cube are regular and hence are of course the largest regular j-simplices contained in the cube. For some additional pairs (j, d), results on the largest *bound* regular j-simplices in a d-cube appear in a paper by Deza and Laurent [DL93]. However, as can be seen from results in Section 5, the largest bound regular simplices in a cube are not necessarily the largest regular simplices. Indeed, it may happen (in contrast to Theorem 1.3) that the largest regular j-simplex in a d-cube has no vertex in common with the cube, and that makes the analysis more difficult.

Aside from the cases in which one of C and K is a cube and the other is a regular simplex, the case in which C and K are both cubes has been considered. The case in which $j = 2$ and $d = 3$ was settled in the late 1700's (see [BC85]). The case in which $j = 3$ and $d = 4$ was studied in [Jo85], and its results were improved in [Lj87], but even this special case has not been completely settled.

I. Weighing Designs

For studying largest j-simplices in Q_d and 0-largest j-simplices in $[-1, 1]^d$, one motivation comes from the theory of weighing designs. Suppose that j objects $O_1, \dots, O_j$ are to be weighed on a spring balance or on a two-pan chemical balance. At least j weighings are required, and greater accuracy can be achieved by increasing the number of weighings. While each weighing can be used to weigh a single object, it was noted by Yates [Ya35] and Hotelling [Ho44] that this is far from optimal, especially when the weights of the objects are small relative to the sensitivity of the balance. Greater accuracy can be obtained by weighing the objects in appropriate combinations, and it is of course desirable to select the combinations that in some sense yield the greatest accuracy.

Suppose (with $j \leqslant d$) that a total of d weighings is permitted, and let each weighing be represented by a row vector of length j. In the case of a spring balance, the ith coordinate of the vector is 0 or 1 according as the ith object O_i is included or omitted in the weighing; the reading of the balance estimates the sum of the weights of the included objects. In the case of a chemical balance, the ith coordinate of the vector is -1, 0, or $+1$ according as the ith object is placed in the left pan, is omitted from the weighing in question, or is placed in the right pan. Standard weights are then added to one pan or the other, to complete the balancing act and thus to estimate the difference between the sum of the weights of the objects on the left pan and the sum of the weights of the objects on the right pan. In each case, the d row vectors may be combined to form a $d \times j$ *design matrix* X in which the ith row represents the ith weighing and the kth column describes the participation of the kth object in the sequence of weighings. Each column belongs to $\{0, 1\}^d$ for the spring balance and to $\{-1, 0, 1\}^d$ for the chemical balance.

As guides to the choice of a weighing design, various optimality criteria have been proposed. The one most thoroughly studied has been the one proposed by Mood [Mo46]. For a given j and d, he calls a design matrix X "best" if X is such that, among all $d \times j$ matrices whose entries all belong to $\{0, 1\}$ (for the spring balance) or to $\{-1, 0, 1\}$ (for the chemical balance), the determinant of the $j \times j$ matrix X^TX is a maximum. The advantage of such an X is that (for the given d) it yields the smallest joint confidence region for the estimated weights (see [Mo46, Ra60] for discussion of this point).

In each case, a design matrix X is best in Mood's sense if and only if its j columns, when taken along with the origin as the vertices of a j-simplex in the appropriate d-cube, produce a 0-largest j-simplex in that cube. For Q_d, finding such a matrix amounts to finding a largest j-simplex in Q^d, for there is always a largest bound j-simplex that has the origin as one of its vertices. In the case of $[-1, 1]^d$, having the origin as a vertex is a real restriction, but it follows from Theorem 2.1 that the maximum value attainable for $\det(XX^T)$ is not reduced when the remaining vertices are required to have exclusively nonzero coordinates. In other words, it may be required that each object participate in each weighing. (This has been noted several times earlier; cf. [Wi46, Co67, GK80b].)

Weighing designs that are "best" in Mood's sense have usually been called *D-optimal* in subsequent publications. There is a rich literature on finding such designs for chemical balances, hence a rich supply of knowledge concerning 0-largest j-simplices in $[-1, 1]^d$ for various pairs (j, d). Ad hoc methods have been used for a number of particular pairs (j, d). However, the most successful overall approach has been the one initiated by Ehlich [Eh64a], developed further by Mitchell [Mi74a,b], and then greatly extended and refined by Galil and Kiefer [GK80a,b,c, GK82a,b]. In addition to these references and the ones mentioned in Section 3, the following papers from our bibliography all contribute to this knowledge: [Ba75, Bh44, BHH81, CC94, CM92, CK85, CKM85, CKM87, Ch80, Ch87, De82, Dy71, FK86, GK83, Ho44, JWM83, KF84, Kh87, Ki45, KKNK94, KKS91, KC83, KS93, MC95, Mo54, MK82, Pa74, Ra59, Ra71, Ra75, SS89, SS89, Tr82, Wh90, Wy70].

Finding D-optimal weighing designs for spring balances amounts to finding largest (unrestricted) j-simplices in d-cubes, while for chemical balances the relevant simplices are required to have a vertex at the center of the cube. From a purely geometric viewpoint, the former problem seems more interesting. However, in contrast to the steady stream of papers related to chemical balances, there has been little concerning spring balances that can be translated directly into results about largest j-simplices in d-cubes. (That fact has been part of the motivation of the present paper.) Since the seminal papers by Hotelling [Ho44] and Mood [Mo46], the most significant work on spring balances appears (from our geometric viewpoint) to be the elegant paper of Jacroux and Notz [JN83], in which they prove that any $b \times v$ design matrix X for which

$$X^TX = (b(v+1)/4v)(I+J)/4v, \qquad \text{if } v \text{ is odd}$$

$$X^TX = (b(v+2)/4(v+1))(I+J), \qquad \text{if } v \text{ is even}$$

is D-optimal over $b \times v$ matrices whose entries are zeros and ones.

In this context, D-optimality corresponds to maximizing the determinant of X^TX. We note that design matrices are transposes of matrices corresponding to simplices in Q_d. We also note that if $X^TX = p(I+J)$ for some p, then X^T is a matrix corresponding to a regular simplex.

See [CK86, WN92] for some more restricted aspects of weighing designs for spring balances.

Research of the first and second authors was supported in part by the National Science Foundation. Research of the second author was also supported in part by the Mittag-Leffler Institute.

We are indebted to J. H. E. Cohn, H. Ehlich, and W. D. Smith for supplying matrices that were used in some of the tests described in Section 3; to MATLAB for some of the determinant computations described in Section 3;

to D. Ljubič for the observation contained in Theorem 4.6; to Mathematica for the symbolic determinant computations that appear in Sections 5–6; to I. Kaplansky and J. J. Seidel for permission to mention the results stated in Section 8E; to J. Kratochvil for reference [Lu87].

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Received 23 January 1995; final manuscript accepted 5 July 1995